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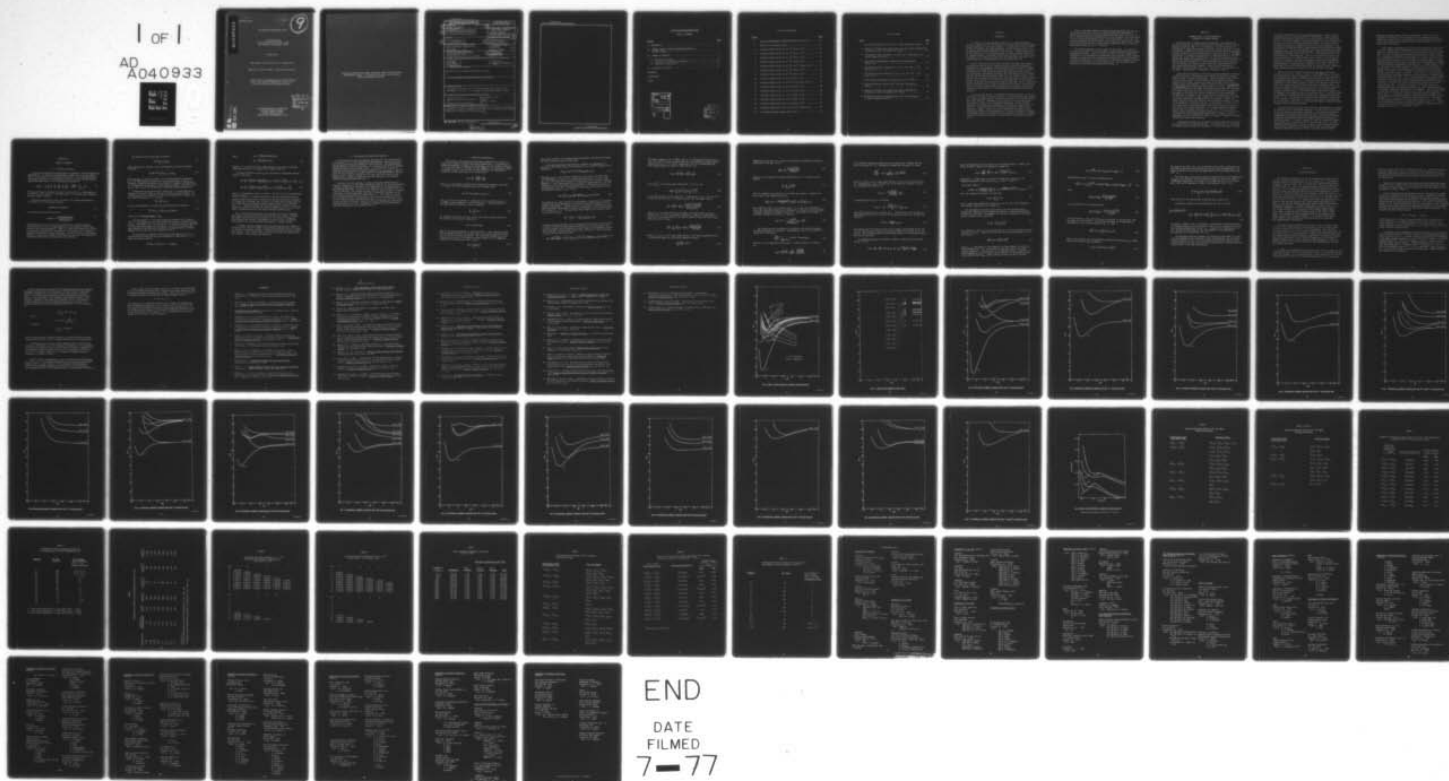
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AIR MOLECULAR COMPUTATION STUDY

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30 March 1977

Final Report for Period June 1976 - January 1977

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This research was supported by the Defense Nuclear  
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19 REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM	
1. REPORT NUMBER AFGL-TR-77-0032	2. GOVT ACCESSION NO.	3. RECIPIENT'S CATALOG NUMBER	
4. TITLE (and Subtitle) AIR MOLECULAR COMPUTATION STUDY	5. TYPE OF REPORT & PERIOD COVERED Final Draft rept. 6/1/76 - 1/30/77		
7. AUTHOR(s) H. Harvey Michels	6. PERFORMING ORG. REPORT NUMBER 1 Jun 76 - 30 Jan 77		
	8. CONTRACT OR GRANT NUMBER(s)		
9. PERFORMING ORGANIZATION NAME AND ADDRESS United Technologies Research Center Silver Lane East Hartford, CT 06108	10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS P.E. 62704H Project No.: Task Work Unit: NA0003		
11. CONTROLLING OFFICE NAME AND ADDRESS Air Force Geophysics Laboratory Hanscom AFB, MA 01731 Contract Monitor: Dr. F. R. Innes/PHR	12. REPORT DATE 30 March 1977		
14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office) 12/59 p.	13. NUMBER OF PAGES 74		
	15. SECURITY CLASS. (of this report) Unclassified		
15a. DECLASSIFICATION/DOWNGRADING SCHEDULE			
16. DISTRIBUTION STATEMENT (of this Report) Approved for public release; distribution unlimited			
17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)			
18. SUPPLEMENTARY NOTES This research was supported by the Defense Nuclear Agency under Subtask S99QAXHD028, Work Unit 37 entitled "Air Molecular Computation Study."			
19. KEY WORDS (Continue on reverse side if necessary and identify by block number) electronic structure      dipole moment function radiative transition probabilities      f-number NO <sup>+</sup> oscillator strength configuration interaction method      NO <sup>++</sup>			
20. ABSTRACT (Continue on reverse side if necessary and identify by block number) Research was directed toward the calculation of the electronic structure and radiative transition probabilities for NO <sup>+</sup> . Ab initio methods, employing the configuration interaction (CI), were utilized.			

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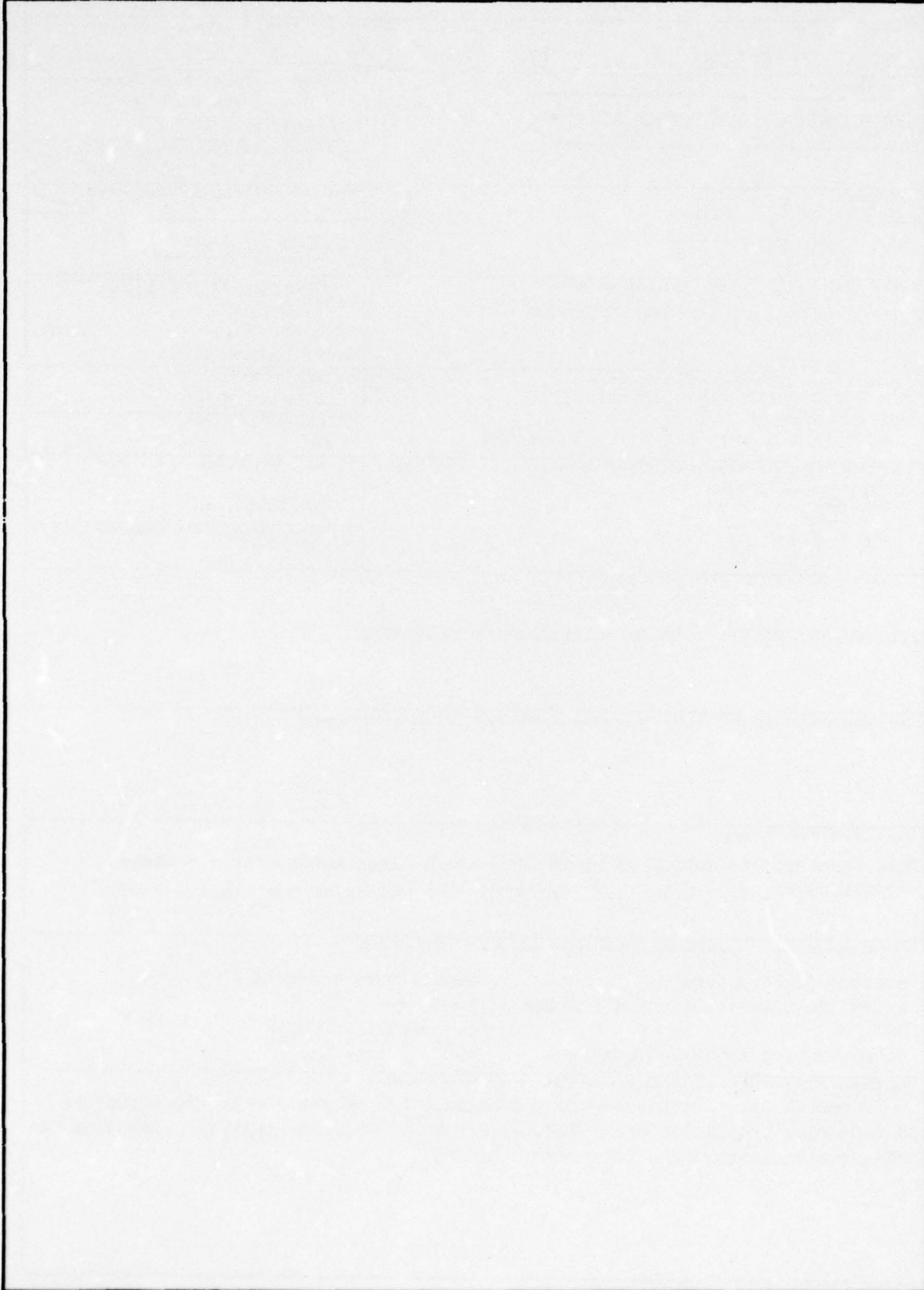
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# Air Molecular Computation Study

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## SECTION I

### INTRODUCTION

The release of certain chemical species into the upper atmosphere results in luminous clouds that display the resonance electronic-vibrational-rotation spectrum of the released species. Such spectra are seen in rocket releases of chemicals for upper atmospheric studies and upon reentry into the atmosphere of artificial satellites and missiles. Of particular interest in this connection is the observed spectra of certain metallic oxides and air diatomic species. From band intensity distribution of the spectra, and knowledge of the f-values for electronic and vibrational transitions, the local conditions of the atmosphere can be determined (Ref. 1).

Present theoretical efforts which are directed toward a more complete and realistic analysis of the transport equations governing atmospheric relaxation and the propagation of artificial disturbances require detailed information of thermal opacities and LWIR absorption in regions of temperature and pressure where molecular effects are important (Refs. 2 and 3). Although various experimental techniques have been employed for both atomic and molecular systems, theoretical studies have been largely confined to an analysis of the properties (bound-bound, bound-free and free-free) of atomic systems (Refs. 4 and 5). This has been due in large part to the unavailability of reliable wavefunctions for diatomic molecular systems, and particularly for excited states or states of open-shell structures. More recently, (Refs. 6-9) reliable theoretical procedures have been prescribed for such systems which have resulted in the development of practical computational programs.

The theoretical analysis of atmospheric reactions requires the knowledge of the electronic structure of atoms, ions and small molecular clusters of nitrogen and oxygen and the interaction of water or other small molecules with these clusters. Knowledge of the chemistry of metal oxide species, which might be present in a contaminated atmosphere, is also desired. Because of the computational complexity for systems with large numbers of electrons, traditional ab initio theoretical methods are difficult and expensive to apply. However, ab initio computational programs based on Slater-type orbitals and incorporating both SCF and configuration interaction analysis have been developed and are available for studies to chemical accuracy for systems such as  $O_2$ ,  $N_2$ , NO and their corresponding molecular ions.

Based on experience gathered through detailed calculations for  $N_2$ ,  $O_2$ , NO and many metal oxide systems, a research program was undertaken to theoretically analyze the low-lying excited molecular states of the  $NO^+$  ion and to calculate transition probabilities for the strongest band systems and for the vibrational-rotational system of the ground state of this ion. The calculated data are presented herein in both transition operator and f-number form to facilitate their use in spectroscopic comparisons and as a basis for collisional studies of the  $N^+ + O$  system.

The general composition of this report is as follows. In Section II, we present a review of the current status of quantum mechanical calculations for molecular systems. This is followed by Section III which deals with a description of the mathematical methods which were employed in this research. Included in Section III are subsections which deal with the construction of electronic wavefunctions, the calculations of expectation properties, and the evaluation of molecular transition probabilities. The calculated results and pertinent discussions are presented in Section IV.



## SECTION II

### CURRENT STATUS OF QUANTUM MECHANICAL METHODS FOR DIATOMIC SYSTEMS

The application of quantum mechanical methods to the prediction of electronic structure has yielded much detailed information about atomic and molecular properties (Ref. 7). Particularly in the past few years, the availability of high-speed computers with large storage capacities has made it possible to examine both atomic and molecular systems using an ab initio approach, wherein no empirical parameters are employed (Ref. 10). Ab initio calculations for diatomic molecules employ a Hamiltonian based on the non-relativistic electrostatic interaction of the nuclei and electrons, and a wavefunction formed by antisymmetrizing a suitable many-electron function of spatial and spin coordinates. For most applications it is also necessary that the wavefunction represent a particular spin eigenstate and that it have appropriate geometrical symmetry. Nearly all the calculations performed to date are based on the use of one-electron orbitals and are of two types: Hartree-Fock or configuration interaction (Ref. 8).

Hartree-Fock calculations are based on a single assignment of electrons to spatial orbitals, following which the spatial orbitals are optimized, usually subject to certain restrictions. Almost all Hartree-Fock calculations have been subject to the assumption that the diatomic spatial orbitals are all doubly occupied, as nearly as possible, and are all of definite geometrical symmetry. These restrictions define the conventional, or restricted, Hartree-Fock (RHF) method (Refs. 11 and 12). RHF calculations can be made with relatively large Slater-type orbital (STO) basis sets for diatomic molecules with first or second-row atoms, and the results are convergent in the sense that they are insensitive to basis enlargement. The RHF model is adequate to give a qualitatively correct description of the electron interaction in many systems, and in favorable cases can yield equilibrium interatomic separations and force constants. However, the double-occupancy restriction makes the RHF method inappropriate in a number of circumstances of practical interest. In particular, it cannot provide potential curves for molecules dissociating into odd-electron atoms (e.g., NO at large internuclear separation), or into atoms having less electron pairing than the original molecule [e.g.,  $O_2 \ ^3\Sigma_g^- \rightarrow O(^3P)$ ]; it cannot handle excited states having unpaired electrons (e.g., the  $^3\Sigma$  state of  $O_2$  responsible for the Schumann-Runge bands); and, in general, it gives misleading results for molecules in which the extent of electron correlation changes with internuclear separation.

Configuration-interaction (CI) methods have the capability of avoiding the limitations of the RHF calculations. If configurations not restricted to doubly-occupied orbitals are included, a CI can, in principle, converge

to an exact wavefunction for the customary Hamiltonian. However, many CI calculations have in fact been based on a restriction to doubly-occupied orbitals and therefore retain many of the disadvantages of the RHF method (Ref. 8). The use of general CI formulations involves three considerations, all of which have been satisfactorily investigated: the choice of basis orbitals, the choice of configurations (sets of orbital assignments), and the specific calculations needed to make wavefunctions describing pure spin states (Ref. 6). The first consideration is the art associated with quantum mechanical electronic structure calculations. Many methods (iterative NSO, perturbation selection, first order CI, etc.) have been advocated for the optimum choice of configurations. There are no firm rules at present and the optimum choice is a strong function of the insight of the particular research investigator. The last consideration, proper spin and symmetry projection, has proved difficult to implement, but computer programs have been developed for linear projection algebra at this Center, and the CI method has been found of demonstrable value in handling excited states and dissociation processes which cannot be treated with RHF techniques.

Either of the above described methods for ab initio calculations reduces in practice to a series of steps, the most important of which are the evaluation of molecular integrals, the construction of matrix elements of the Hamiltonian, and the optimization of molecular orbitals (RHF) or configuration coefficients (CI). For diatomic molecules, these steps are all comparable in their computing time, so that a point has been reached where there is no longer any one bottleneck determining computation speed. In short, the integral evaluation involves the use of ellipsoidal coordinates and the introduction of the Neumann expansion for the interelectronic repulsion potential (Ref. 13); the matrix element construction depends upon an analysis of the algebra of spin eigenfunctions (Ref. 14); and the orbital or configuration optimization can be carried out by eigenvalue techniques (Refs. 15, 16). All the steps have by now become relatively standard, and can be performed efficiently on a computer having 32,000 to 65,000 words of core storage, a cycle time in the microsecond range, and several hundred thousand words of peripheral storage.

Both the RHF and CI methods yield electronic wavefunctions and energies as a function of the internuclear separation, the RHF method for one state, and the CI method for all states considered. The electronic energies can be regarded as potential curves, from which may be deduced equilibrium internuclear separations, dissociation energies, and constants describing vibrational and rotational motion (including anharmonic and rotation-vibration effects). It is also possible to solve the Schrödinger equation for the motion of the nuclei subject to the potential curves, to obtain vibrational wavefunctions for use in transition probability calculations. The electronic wavefunctions themselves can be used to estimate dipole moments of individual electronic states, transition moments between

different electronic states, and other properties. While all of the calculations described in this paragraph have been carried out on some systems, the unavailability of good electronic wavefunctions and potential curves has limited actual studies of most of these properties to a very small number of molecules.

A few studies illustrating the scope of the current work in this field are cited. Exhaustive RHF calculations have been reported for first and second-row hydrides (Refs. 17 and 18) for most first-row diatomic molecules (Ref. 19), and for many other molecules containing second-row atoms (Ref. 20). Configuration-interaction calculations restricted to double occupancy are illustrated by the work of Das and Wahl on  $\text{Li}_2$  and  $\text{F}_2$  (Refs. 8 and 21). They determined an optimum choice of orbitals for a small number of configurations designed to permit proper description of the dissociation products, and obtained highly satisfactory potential curves. Davidson (Refs. 22 and 23) has carried out doubly occupied CI studies with very large numbers of configurations to gain more insight into the description of correlation energy. The largest of the CI studies not restricted to doubly occupied orbitals have been carried out at UTRC. The 62 states of  $\text{O}_2$  dissociating into low-lying atomic oxygen states have been described in a qualitatively consistent manner (Ref. 24). Many of these states involve several unpaired electrons, and the success of the treatment depended critically upon the inclusion of all types of pertinent configurations and upon proper handling of the spin. Similar work on the 102 low-lying  $\text{N}_2$  states has now been completed (Ref. 25). In striking contrast to the recent progress in obtaining electronic energies and wavefunctions, rather few calculations of electronic transition moments have been attempted. Among the few studies in this area is the work of Michels on  $\text{He H}^+$  (Ref. 26) and of Henneker and Popkie (Ref. 27) on diatomic hydrides using Hartree-Fock wavefunctions. More recently a theoretical program for calculating band strengths for the systems  $\text{N}_2$  (1 PS),  $\text{O}_2$  (SR), and  $\text{NO}$  ( $\beta$ ) has been carried out. The results of this program indicate that reliable band strengths (10 to 25 percent) can be calculated, provided a CI approach is employed (Ref. 28). Similar work has been performed for band-to-band transition probabilities for the systems  $\text{LiO}$ ,  $\text{AlO}$ ,  $\text{FeO}$ ,  $\text{UO}$ ,  $\text{UO}^+$  and  $\text{TiO}$  (Ref. 29).



## SECTION III

### METHOD OF APPROACH

#### A. Electronic Structure

A spin-free nonrelativistic Hamiltonian is employed in the Born-Oppenheimer approximation. In systems containing atoms as heavy as N or O, this approximation is quite good for low-lying molecular states. For a diatomic molecule containing  $n$  electrons, the approximation leads to an electronic Hamiltonian depending parametrically on the internuclear separation  $R$ :

$$\mathcal{H}(R) = -\frac{1}{2} \sum_{i=1}^n \nabla_i^2 - \sum_{i=1}^n \frac{Z_A}{r_{iA}} - \sum_{i=1}^n \frac{Z_B}{r_{iB}} + \frac{Z_A Z_B}{R} + \sum_{i>j}^n \frac{1}{r_{ij}} \quad (1)$$

where  $Z_A$  and  $Z_B$  are the charges of nuclei A and B, and  $r_{iA}$  is the separation of electron  $i$ , and nucleus A. The Hamiltonian  $H$  is in atomic units (energy in Hartrees, length in Bohrs).

Electronic wavefunctions,  $\psi(R)$ , are made to be optimum approximations to solutions of the Schrodinger equation

$$\mathcal{H}(R)\psi(R) = E(R)\psi(R) \quad (2)$$

by invoking the variational principle

$$\delta W(R) = \delta \frac{\int \psi^*(R) \mathcal{H}(R) \psi(R) d\tau}{\int \psi^*(R) \psi(R) d\tau} \quad (3)$$

The integrations in Eq. (3) are over all electronic coordinates and the stationary values of  $W(R)$  are approximations to the energies of states described by the corresponding  $\psi(R)$ . States of a particular symmetry are studied by restricting the electronic wavefunction to be a projection of the appropriate angular momentum and spin operators. Excited electronic states corresponding to a particular symmetry are handled by construction of configuration interaction wavefunctions of appropriate size and form.

The specific form for  $\psi(R)$  may be written

$$\Psi(R) = \sum_{\mu} c_{\mu} \Psi_{\mu}(R) \quad (4)$$

where each  $\Psi_{\mu}(R)$  is referred to as a configuration, and has the general structure

$$\Psi_{\mu}(R) = \mathcal{A} \mathcal{O}_S \prod_{i=1}^n \psi_{\mu i}(\mathbf{r}_i, R) \theta_M \quad (5)$$

where each  $\psi_{\mu i}$  is a spatial orbital,  $\mathcal{A}$  is the antisymmetrizing operator,  $\mathcal{O}_S$  is the spin-projection operator for spin quantum number  $S$ , and  $\theta_M$  is a product of  $\alpha$  and  $\beta$  one-electron spin functions of magnetic quantum number  $M$ . No requirement is imposed as to the double occupancy of the spatial orbital, so Eqs. (4) and (5) can describe a completely general wavefunction.

In Hartree-Fock calculations  $\psi$  is restricted to a single  $\psi_{\mu}$  which is assumed to consist as nearly as possible of doubly-occupied orbitals. The orbitals  $\psi_{\mu i}$  are then selected to be the linear combinations of basis orbitals best satisfying Eq. (3). Writing

$$\psi_{\mu i} = \sum_{\nu} a_{\nu i} \chi_{\nu} \quad (6)$$

The  $a_{\nu i}$  are determined by solving the matrix Hartree-Fock equations

$$\sum_{\nu} F_{\lambda \nu} a_{\nu i} = \epsilon_i \sum_{\nu} S_{\lambda \nu} a_{\nu i} \quad (\text{each } \lambda) \quad (7)$$

where  $\epsilon_i$  is the orbital energy of  $\psi_{\mu i}$ .

The Fock operator  $F$  has been thoroughly discussed in the literature (Ref. 31) and depends upon one- and two-electron molecular integrals and upon the  $a_{\nu i}$ . This makes Eq. (7) nonlinear and it is therefore solved iteratively. UTRC has developed programs for solving Eq. (7) for both closed and open-shell systems, using basis sets consisting of Slater-type atomic orbitals. Examples of their use are in the literature (Ref. 6).

In configuration interaction calculations, the summation in Eq. (4) has more than one term, and the  $c_{\mu}$  are determined by imposing Eq. (3), to obtain the secular equation

$$\sum_{\nu} (H_{\mu \nu} - W S_{\mu \nu}) c_{\nu} = 0 \quad (\text{each } \mu) \quad (8)$$

where

$$H_{\mu\nu} = \int \Psi_{\mu}^*(R) \mathcal{H}(R) \Psi_{\nu}(R) d\tau$$

$$S_{\mu\nu} = \int \Psi_{\mu}^*(R) \Psi_{\nu}(R) d\tau \quad (9)$$

Equation (7) is solved by matrix diagonalization using either a modified Givens method (Ref. 15) or a method due to Shavitt (Ref. 16).

The matrix elements  $H_{\mu\nu}$  and  $S_{\mu\nu}$  may be reduced by appropriate operator algebra to the forms

$$H_{\mu\nu} = \sum_P \epsilon_P \left\langle \theta_M \left| \mathcal{O}_S P \right| \theta_M \right\rangle \left\langle \prod_{i=1}^n \Psi_{\mu_i}(\underline{r}_i, R) \left| \mathcal{H}(R) P \right| \prod_{i=1}^n \Psi_{\nu_i}(\underline{r}_i, R) \right\rangle \quad (10)$$

$$S_{\mu\nu} = \sum_P \epsilon_P \left\langle \theta_M \left| \mathcal{O}_S P \right| \theta_M \right\rangle \left\langle \prod_{i=1}^n \Psi_{\mu_i}(\underline{r}_i, R) \left| P \right| \prod_{i=1}^n \Psi_{\nu_i}(\underline{r}_i, R) \right\rangle \quad (11)$$

where  $P$  is a permutation and  $\epsilon_P$  its parity. The sum is over all permutations.  $\langle \theta_M | \mathcal{O}_S P | \theta_M \rangle$  is a "Sanibel coefficient" and the remaining factors are spatial integrals which can be factored into one- and two-electron integrals. If the  $\Psi_{\mu_i}$  are orthonormal, Eqs. (10) and (11) become more tractable and the  $H_{\mu\nu}$  and  $S_{\mu\nu}$  may be evaluated by explicit methods given in the literature (Ref. 14). Computer programs have been developed for carrying out this procedure, and they have been used for problems containing up to 40 total electrons, 10 unpaired electrons, and several thousand configurations.

The CI studies described above can be carried out for any orthonormal set of  $\Psi_{\mu_i}$  for which the molecular integrals can be calculated. Programs developed by UTRC made specific provision for the choice of the  $\Psi_{\mu_i}$  as Slater-type atomic orbitals, as symmetry molecular orbitals, as Hartree-Fock orbitals, or as more arbitrary combinations of atomic orbitals.

In summary, computer programs have been developed which are capable of carrying out all the steps needed to make diatomic Hartree-Fock or CI studies for closed- or open-shell systems, including excited states, based on Slater-type orbitals. These studies lead to electronic energies and wavefunctions as a function of the internuclear separation.



## B. Vibrational and Rotational Properties

For an electronic state described by  $\psi(R)$  and  $W(R)$ , the relative motion of the nuclei is, in the Born-Oppenheimer approximation, subject to a potential having at internuclear separation  $R$  the value  $W(R)$ . By considering the quantum mechanics of the nuclear motion, it is possible from  $W(R)$  to calculate vibrational and rotational energy levels. It is convenient to report the vibration-rotation structure in terms of parameters  $r_e$ ,  $D_e$ ,  $\omega_e x_e$ ,  $B_e$ ,  $\alpha_e$ , etc., which are also available by standard reduction of experimental data. Such an analysis can be routinely carried out for bound electronic states, using a Dunham analysis computer program which has been deposited in the Quantum Chemistry Program Exchange (QCPE 113).

From  $W(R)$  it is also possible to obtain vibrational wavefunctions by numerical integration of the radial Schrodinger equation for the nuclear motion. A computer program which carried out this calculation by the Numerov procedure has been developed. Any  $W(R)$  can be handled since the program fits it by a spline technique. This program has been used for several years on a variety of problems; a typical application has been to excitation transfer in collisions of normal and metastable He atoms (Ref. 30). The input  $W(R)$  can be the calculated potential corresponding to the electronic wavefunctions ( $R$ ) or it can be derived using an RKR procedure (Refs. 31 and 32). The input can be either the basic  $B(v)$  and  $G(v)$  data or the derived experimental spectroscopic constants based on this data. Programs for implementing the RKR procedure have been described in the literature (Ref.33).

### C. Transition Probabilities

The electronic and vibrational-rotational wavefunctions of a pair of states can be used to calculate transition probabilities. If two molecular states are separated in energy by an amount  $\Delta E_{nm} = h\nu$  ( $h$  = Planck's constant,  $c$  = velocity of light,  $\nu$  = frequency in wave numbers), the semiclassical theory of radiation (Refs. 34 and 35) yields for the probability of a spontaneous transition from an upper state  $n$  to a lower state  $m$

$$A_{nm} = \frac{4}{3} \frac{\Delta E_{nm}^3}{\hbar^4 c^3} \frac{S_{nm}}{g_n} \quad (12)$$

Here  $A_{nm}$  is the Einstein coefficient for spontaneous transition from level  $n \rightarrow m$ ,  $g_n$  is the total degeneracy factor for the upper state

$$g_n = (2 - \delta_{\sigma, \Lambda'}) (2S' + 1) (2J' + 1) \quad (13)$$

and  $S_{nm}$  is the total strength of a component line in a specific state of polarization and propagated in a fixed direction. A related quantity is the mean radiative lifetime of state  $n$  defined by

$$\frac{1}{\tau_n} = \sum_{m < n} A_{nm} \quad (14)$$

the summation being over all lower levels which offer allowed connections. The intensity of the emitted radiation is

$$I_{nm} = \Delta E_{nm} N_n A_{nm} \quad (15)$$

where  $N_n$  is the number density in the upper state  $n$ . This analysis assumes that all degenerate states at the same level  $n$  are equally populated, which will be true for isotropic excitation. The total line strength  $S_{nm}$  can be written as the square of the transition moment summed over all degenerate components of the molecular states  $n$  and  $m$ :

$$S_{nm} = \sum_{i,j} |M_{ji}|^2 \quad (16)$$

where  $j$  and  $i$  refer to all quantum numbers associated collectively with upper and lower electronic states, respectively.

In the Born-Oppenheimer approximation, assuming the separability of electronic and nuclear motion, the wavefunction for a diatomic molecule can be written as

$$\psi'_{vJM\Lambda} = \psi'_{el}(\underline{r}, R) \psi_v(R) \psi_{JM\Lambda}(\theta, \chi, \phi) \quad (17)$$

where  $\psi'_{el}(\underline{r}, R)$  is an electronic wavefunction for state  $i$  at fixed internuclear separation  $R$ ,  $\psi_v(R)$  is a vibrational wavefunction for level  $v$  and  $\psi_{JM\Lambda}(\theta, \chi, \phi)$  refers to the rotational state specified by electronic angular momentum  $\Lambda$ , total angular momentum  $J$  and magnetic quantum number  $M$ . The representation is in a coordinate system related to a space-fixed system by the Eulerian angles  $(\theta, \chi, \phi)$ . The transition moment  $M_{ji}$  can be written, using the wavefunction given by Eq. (17), as

$$M_{ji} = \int \psi_{v', J', \Lambda', M'}^j \{ \underline{M}^e + \underline{M}^n \} \psi_{v'', J'', \Lambda'', M''}^i d\tau_e d\tau_v d\tau_r \quad (18)$$

The subscripts  $e$ ,  $v$  and  $r$  refer to the electronic, vibrational and rotational wavefunctions and  $\underline{M}^e$  and  $\underline{M}^n$  are the electronic and nuclear electric dipole moments, respectively. Integration over the electronic wavefunction, in the Born-Oppenheimer approximation, causes the contribution of the nuclear moment  $\underline{M}^n$  to vanish for  $i = j$ . The electronic dipole moment can be written (Refs. 35 and 36) in the form

$$\underline{M}^e = -\sum_k e \underline{r}'_k = -\left\{ \sum_k e \underline{r}_k \right\} \cdot \underline{\mathcal{D}}(\theta, \chi, \phi) \quad (19)$$

where the primed coordinates refer to the space fixed system, the coordinates  $\underline{r}_k$  refer to a molecule-fixed system and  $\underline{\mathcal{D}}(\theta, \chi, \phi)$  is a group rotation tensor whose elements are the direction cosines related to the Eulerian rotation angles  $(\theta, \chi, \phi)$ . Using bracket notation, Eqs. (18) and (19) can be combined to yield for the transition moment

$$M_{ji} = M_{iv'' J'' \Lambda'' M''}^{jv' J' \Lambda' M'} = \left\langle jv' \left| -\sum_k e \underline{r}_k \right| iv'' \right\rangle \cdot \left\langle J' \Lambda' M' \left| \underline{\mathcal{D}}(\theta, \chi, \phi) \right| J'' \Lambda'' M'' \right\rangle \quad (20)$$



The matrix elements  $\langle J' \Lambda' M' | \mathcal{D}(\theta, \chi, \phi) | J'' \Lambda'' M'' \rangle$  determine the group selection rules for an allowed transition and have been evaluated for many types of transitions (Refs. 37, 38 and 39) Summing Eq. (20) over the degenerate magnetic quantum numbers  $M'$  and  $M''$  we have from Eq. (16)

$$S_{nm} = S_{m v'' J'' \Lambda''}^{n v' J' \Lambda'} = S_{J'' \Lambda''}^{J' \Lambda'} \rho_{m v''}^{n v'} \quad (21)$$

where  $S_{J'' \Lambda''}^{J' \Lambda'}$  is the Honl-London factor (Refs. 40 and 41) and

$$\rho_{m v''}^{n v'} = \sum_{i,j} \left| \left\langle j v' \left| -\sum_k e r_k \right| i v'' \right\rangle \right|^2 \quad (22)$$

is the band strength for the transition. Combining Eqs. (13), (15) and (21), we have for the intensity of a single emitting line from upper level  $n$ :

$$I_{nm} = I_{m v'' J''}^{n v' J'} = \frac{4}{3} N_{J'} \frac{[\Delta E_{m v'' J''}^{n v' J'}]^4 S_{m v'' J'' \Lambda''}^{n v' J' \Lambda'}}{\hbar^4 c^3 \omega_n (2J' + 1)} \quad (23)$$

where  $N_{J''}$  is the number density in the upper rotational state  $J'$  and  $\omega_n = (2 - \delta_{\sigma, \Lambda}) (2S' + 1)$  is the electronic degeneracy. Taking an average value of  $E_{m v'' J''}^{n v' J'}$  for the whole band, Eq. (23) can be summed to yield the total intensity in the  $(v', v'')$  band:

$$I_{m v''}^{n v'} = \sum_{J', J''} I_{m v'' J''}^{n v' J'} = \frac{4}{3} N_{v'} \frac{[\overline{\Delta E_{m v''}^{n v'}}]^4 \rho_{m v''}^{n v'}}{\hbar^4 c^3 \omega_n} \quad (24)$$

where  $N_{v'} = \sum_{J'} N_{J'}$  is the total number density in the upper vibrational level  $v'$  and where we make use of the group summation property

$$\sum_{J''} S_{J'' \Lambda''}^{J' \Lambda'} = (2J' + 1) \quad (25)$$

Comparing Eq. (15) and (24), we have for the Einstein spontaneous transition coefficient of the band ( $v', v''$ )

$$A_{mv''}^{nv'} = \frac{4}{3} \frac{[\Delta E_{mv''}^{nv'}]^3 p_{mv''}^{nv'}}{\hbar^4 c^3 \omega_n} \quad (26)$$

Similarly, the lifetime of an upper vibrational level  $v'$  of state  $n$  can be written

$$\frac{1}{\tau_n} = \sum_{m < n} \sum_{v''} A_{mv''}^{nv'} \quad (27)$$

where the summation runs over all  $v''$  for each lower state  $m$ . Equation (26) can be cast in the computational form

$$A_{mv''}^{nv'} (\text{sec}^{-1}) = \frac{(21.41759 \times 10^9)}{\omega_n} [\Delta E_{mv''}^{nv'} (\text{a.u.})]^3 p_{mv''}^{nv'} (\text{a.u.}) \quad (28)$$

where  $\Delta E_{mv''}^{nv'}$  and  $p_{mv''}^{nv'}$  are in atomic units. It is also often convenient to relate the transition probability to the number of dispersion electrons needed to explain the emission strength classically. This number, the  $f$ -number or oscillator strength for emission, is given by

$$f_{nm, v'v''} = \frac{mc^3 h^2}{2e^2 [\Delta E_{mv''}^{nv'}]^2} A_{mv''}^{nv'} \quad (29)$$

The inverse process of absorption is related to the above development through the Einstein B coefficient. Corresponding to Eq. (15), we have for a single line in absorption

$$\frac{I_{mn}}{I_0 \Delta x} = \int_{\text{line}(v''v'J''J')} K(\nu) d\nu = h\nu_{mn} N_m B_{mn} \quad (30)$$

where  $K(\nu)$  is the absorption coefficient of a beam of photons of frequency and

$$B_{mn} = B_{mv''J''\Lambda''}^{nv'J'\Lambda'} = \frac{2\pi}{3\hbar^2 c} \frac{S_{mv''J''\Lambda''}^{nv'J'\Lambda'}}{\omega_m (2J''+1)} \quad (31)$$

is the Einstein absorption coefficient for a single line. Summing over all lines in the band ( $v''$ ,  $v'$ ), assuming an average band frequency, we obtain

$$\frac{I_{m\nu}^{nv'}}{I_0^0 \Delta x} = N_{v''} \frac{2\pi}{3\hbar^2 c \omega_m} \rho_{m\nu}^{nv'} \overline{\Delta E}_{m\nu}^{nv'} \quad (32)$$

where  $N_{v''} = \sum_{J''} N_{J''}$  is the total number density in the lower vibrational state  $v''$ . Corresponding to Eqs. (28) and (29) we can define an f-number or oscillator strength for absorption as

$$f_{mn, v''v'} = \frac{2m}{3\hbar^2 e^2 \omega_m} \overline{\Delta E}_{m\nu}^{nv'} \rho_{m\nu}^{nv'} \quad (33)$$

In computational form, Eq. (33) becomes

$$f_{mn, v''v'} = \frac{2}{3} \cdot \frac{\overline{\Delta E}_{m\nu}^{nv'} (\text{a.u.})}{\omega_m} \rho_{m\nu}^{nv'} (\text{a.u.}) \quad (34)$$

where  $\overline{\Delta E}_{m\nu}^{nv'}$  and  $\rho_{m\nu}^{nv'}$  are in atomic units. Combining Eqs. (26) and (29) and comparing with Eq. (33), we see that the absorption and emission f-numbers are related by

$$f_{mn, v''v'} = \left( \frac{\omega_n}{\omega_m} \right) f_{nm, v'v''} \quad (35)$$

Some caution must be observed in the use of f-numbers given either by Eq. (29) or (33) since both band f-numbers and system f-numbers are defined in the literature. The confusion arises from the several possible band averaging schemes that can be identified.

An integrated absorption coefficient (density corrected) can be defined from Eq. (32) as

$$S_{v'', v'} = \frac{1}{P_c} I_{m\nu}^{nv'} = N_{v''} B_{v'', v'} \left( 1 - \exp \frac{-hc\nu_{v'', v'}}{kT} \right) \frac{h\nu_{v'', v'}}{P_c^2} \quad (36)$$



where the exponential factor corrects for stimulated emission. Equation (36) can be written in terms of the absorption f-number as

$$S_{v'',v'} = \frac{\pi e^2}{mc^2} \frac{N_{v''}}{P} \left( 1 - \exp \frac{-hc\nu_{v'',v'}}{kT} \right) f_{mn,v''v'} \quad (37)$$

Using  $hvc/k = 1.43880 \text{ cm-K}^0$ , we obtain a computational formula for the integrated absorption coefficient as  $S_{v'',v'} (\text{cm}^{-2} \cdot \text{atm}^{-1}) =$

$$S_{v'',v'} (\text{cm}^{-2} \text{ atm}^{-1}) = 2.3795 \times 10^7 \left( \frac{273.16}{T(\text{K}^0)} \right) \left( \frac{N_{v''}}{N_T} \right) \left( 1 - \exp \frac{1.43880 \nu_{v'',v'} (\text{cm}^{-1})}{T} \right) \cdot f_{mn,v''v'} \quad (38)$$

The total integrated absorption is found from

$$S_{\text{TOTAL}} = \sum_{v''} \sum_{v'} S_{v'',v'} \quad (39)$$

where, under normal temperature conditions, only the first few fundamentals and overtones contribute to the summations.

The developments given above are rigorous for band systems where an average band frequency can be meaningfully defined. Further approximations, however, are often made. For example, the electronic component of the dipole transition moment can be defined as

$$R_{ji}(R) = \left\langle j \left| -\sum_k e r_k \right| i \right\rangle \quad (40)$$

This quantity is often a slowly varying function of  $R$  and an average value can sometimes be chosen. Equation (22) can then be written approximately in factored form as

$$p_{mv''}^{nv'} \approx q_{v'v''} \sum_{i,j} \left| \bar{R}_{ji}(\bar{R}) \right|^2 \quad (41)$$

where  $q_{v'v''}$ , the square of the vibrational overlap integral, is called the Franck-Condon factor.  $R_{ji}$  is evaluated at some mean value of the internuclear separation  $R$ . In addition, it is sometimes possible to account for a weak  $R$ -dependence in  $M^e$  by a Taylor series expansion of this quantity about some reference value,  $R_{\alpha\beta}$ , usually referred to the (0,0) band. We have

$$R_{ji} \approx R_{ji}^{\alpha\beta} \left[ 1 + a(R - R_{\alpha\beta}) + b(R - R_{\alpha\beta})^2 + \dots \right] \quad (42)$$

Substituting into Eq. (22) and integrating yields

$$p_{mV'}^{nV'} \approx q_{V'V''} \sum_{i,j} \left| R_{ji}^{\alpha\beta} \left[ 1 + a(\bar{R}_{V'V''} - R_{\alpha\beta}) + b(\bar{R}_{V'V''} - R_{\alpha\beta})^2 + \dots \right] \right|^2 \quad (43)$$

where

$$(\bar{R}_{V'V''} - R_{\alpha\beta}) = \frac{\langle V' | (R - R_{\alpha\beta}) | V'' \rangle}{\langle V' | V'' \rangle} \quad (44)$$

is the R-centroid for the transition and

$$(\bar{R}_{V'V''} - R_{\alpha\beta})^2 = \frac{\langle V' | (R - R_{\alpha\beta})^2 | V'' \rangle}{\langle V' | V'' \rangle} \quad (45)$$

is the  $R^2$ -centroid. Note that this last term differs (to second order) from the square of the R-centroid. An alternate procedure can be developed by evaluating Eq. (40) at each R-centroid,  $R_{V'V''}$ . Then

$$p_{mV''}^{nV'} \approx q_{V'V''} \sum_{i,j} \left| R_{ji}(R_{V'V''}) \right|^2 \quad (46)$$

Equation (46) assumes that the vibrational wavefunction product  $\psi_{V'}, \psi_{V''}$  behaves like a delta function upon integration,

$$\psi_{V'} \psi_{V''} = \delta(R - \bar{R}_{V'V''}) \langle V' | V'' \rangle \quad (47)$$

The range of validity of Eq. (46) is therefore questionable, particularly for band systems with bad overlap conditions such as oxygen Schumann-Runge. The range of validity of the R-centroid approximation has been examined by Frazer (Ref. 42).

The final step in calculating transition probabilities is the determination of  $R_{ji}(R)$ , the electronic dipole transition moment, for the entire range of internuclear separations,  $R$ , reached in the vibrational levels to be considered. This can be expressed in terms of the expansion of Eq. (4) as

$$R_{ji}(R) = \sum_{\mu\nu} c_{\mu}^j c_{\nu}^i \langle \psi_{\mu}(R) | \underline{M}^e | \psi_{\nu}(R) \rangle \quad (48)$$

where  $c_{\mu}^j$  and  $c_{\nu}^i$  are coefficients for  $\psi_{el}^j$  and  $\psi_{el}^i$ , respectively.

An analysis similar to that yielding Eqs. (10) and (11) gives

$$\langle \psi_{\mu}(R) | \underline{M}^e | \psi_{\nu}(R) \rangle = \sum_p \epsilon_p \langle \theta_{Ms} | O_{Sp} | \theta_{Ms} \rangle \left\langle \prod_{k=1}^n \psi_{\mu k}(r_k, R) \right| \underline{M}^e P \left| \prod_{k=1}^n \psi_{\nu k}(r_k, R) \right\rangle \quad (49)$$

The spatial integral in Eq. (49) reduces to one-electron integrals equivalent to overlap integrals, and the evaluation of Eq. (49) can be carried out by the same computer programs used for Eq. (11). Programs for evaluating  $R_{ji}(R)$  in Eq. (48) have been developed at UTRC and examples of their application have appeared in the literature (Ref. 26).

For perturbed electronic systems, the transition dipole moment will have a strong  $R$ -dependence and  $R$ -centroid or other approximations will be invalid. A direct evaluation of Eq. (22) would therefore be required using the fully-coupled system of electronic and vibrational wavefunctions to properly account for the source of the band perturbations.



## SECTION IV

### DISCUSSION OF RESULTS

The absorption coefficient for the  $\text{NO}^+$  fundamental vibration-rotation band has recently been measured by Bien, et al. (Ref. 43). The reported integrated value is  $140 \text{ cm}^{-2} \text{ atm}^{-1}$  in conflict with previous experimental estimates of  $500 \text{ cm}^{-2} \text{ atm}^{-1}$  (Ref. 44) and a recent theoretical value of  $89 \text{ cm}^{-2} \text{ atm}^{-1}$  (Ref. 45). Since the dominant atmospheric molecular ion above 100 km is  $\text{NO}^+$ , its radiation characteristics and interactions with electrons and other atomic and molecular species are of primary importance in understanding the detailed chemistry of the atmosphere. Relatively little is known about the excited electronic states of the  $\text{NO}^+$  ion. Accurate potential curves are available for the ground  $X^1\Sigma^+$  state and for the  $A^1\Pi$  and a  $3\Sigma^+$  excited states of  $\text{NO}^+$  (Ref. 46). Gilmore also gives some experimental estimates of other excited states of  $\text{NO}^+$ . More recently Thulstrup, et al. (Refs. 47 and 48) have assigned additional excited states of  $\text{NO}^+$  based on photoelectron spectrum. A summary of these data is shown in Fig. 1. A correlation diagram for some of the low-lying valence excited states of  $\text{NO}^+$  is shown in Table I. In addition to these valence excited states there exists a large manifold of Rydberg states to the  $\text{N}^+(3P) + \text{O}^+(4S)$  limit. The energies of the dissociation limits of the low-lying electronic states of  $\text{NO}^+$  are shown in Table 2. It is obvious that only a small fraction of the low-lying excited states for this system have been experimentally investigated.

Few theoretical studies have been carried out for the excited states of this system. Lefebvre-Brion and Moser (Refs. 49 and 50) have studied the lowest-lying  $1\Pi$  and  $3\Pi$  states in an SCF framework. More recently, Thulstrup and Öhrn (Refs 47 and 48) have examined low-lying singlet and triplet states of  $\Sigma^+$ ,  $\Sigma^-$ ,  $\Pi$  and  $\Delta$  symmetry. Their studies excluded higher spin and angular momentum states which may be important in perturbation analysis. Also, their calculations for  $3\Pi$ ,  $1\Sigma$  and  $3\Sigma$  symmetries were truncated in expansion length owing to their computer program limitations. Their predicted locations for these states are not in good agreement with the best experimental estimates.

A complete and quantitatively uniform ab initio CI study of all the low-lying valence states of  $\text{NO}^+$  was carried out as part of the research conducted under this program. This study was similar to that carried out for the 102 low-lying valence states of the nitrogen molecule (Ref. 25). Many of the

states are similar since  $\text{NO}^+$  is isoelectronic with  $\text{N}_2$ . Empirically adjusted potential energy curves, based on both the ab initio calculations and the available experimental spectroscopic data, have been derived and studies of the radiation characteristics of the strongest electronic transitions have been carried out.

Figures 2-17 illustrates the low-lying valence state potential energy curves for the  $\text{NO}^+$  system. These curves have been calculated using a full CI within a minimum STO basis. The configuration sizes and number of states calculated are shown in Table 3.

These calculations have the property of correct dissociation to atomic limits and, as previously found for the  $\text{N}_2$  system, a gradual and uniformly increasing correlation error with decreasing internuclear separation. This error arises from inadequacy of the basis set to fully describe polarization effects between the core and valence electrons. This error is quantitatively similar for the excited low-lying states of a given symmetry and our calculated potential curves have therefore been empirically adjusted to yield agreement with RKR curves constructed from the limited known spectroscopic data. This empirical adjustment takes the form:

$$\Delta E(R) = E(R)_{\text{calc.}} - E(R)_{\text{exp.}}$$

We find that  $\Delta E$  is a strongly increasing function of  $R$  for short internuclear separations but is nearly independent of the spin state and only weakly dependent of the angular momentum of the excited states. Thus a nearly universal correction curve (error  $\sim .2$  eV) exists for most of the  $\text{NO}^+$  system of valence excited states.

Our summary of known experimental spectroscopic data for the low-lying bound valence states of  $\text{NO}^+$  is given in Table 4. The corresponding potential curves are given in Fig. 1. The most interesting curves from the standpoint of the charge transfer reaction are those of  $^5\Sigma^+$  and  $^5\Pi$  symmetry. An avoided crossing between  $^5\Sigma^+$  I and  $^5\Sigma^+$  II is apparent and this could be the most important charge transfer channel. Another observation is that the  $^5\Pi$  I state connecting with  $\text{N}^+ + \text{O}$  crosses the  $^5\Sigma^+$  I connecting to  $\text{N} + \text{O}^+$  at or near the dissociation limit of  $\text{N}^+ + \text{O}$ . This means that a large low-energy ( $< .5$  eV) cross-section may be found for this reaction. Further studies of these symmetries are indicated.

We have carried out an analysis of the vibrational-rotational radiation/absorption characteristics for the ground  $X^1\Sigma^+$  state of  $\text{NO}^+$ . Calculated oscillator strengths for the vibrational-rotational system are given in Table 5. The corresponding calculated Einstein coefficients are given in Table 6. These are based on the calculated dipole moment function. This function is similar to that given by Billingsley (Ref. 45) but exhibits a somewhat steeper slope near the equilibrium separation of the ion. The long range behavior of the dipole moment function for  $\text{N} + \text{O}^+$  can be written as

$$\mu(R) \rightarrow + \frac{R}{2} - 16 \text{ z c.m.} \\ R \rightarrow \infty$$

where

$$\text{z c.m.} = \left[ \frac{1}{2} - \frac{M_N}{M_N + M_O} \right] R$$

therefore,

$$\mu(R) \rightarrow -.0311933 R \\ R \rightarrow \infty$$

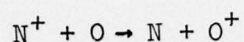
Here the dipole moment is defined relative to a center-of-mass coordinate system and we note that  $\mu(R)$  is not gauge-invariant for an ionized system.

This dipole moment functions yields somewhat higher integrated band absorption coefficients than those reported by Billingsley. Our calculated value for the fundamental band is  $168 \text{ cm}^{-2} \text{ atm}^{-1}$  which can be compared with an experimental lower bound ( $> 140 \text{ cm}^{-2} \text{ atm}^{-1}$ ) as reported by Bien et al. (Ref. 43). A complete summary of the calculated integrated absorption coefficients is given in Table 7.

The  $\text{NO}^{++}$  system is illustrated in Fig. 18 using the data of Thulstrup, et al. (Ref. 48). A correlation diagram for the low-lying valence excited states of  $\text{NO}^{++}$  is shown in Table 8. The energies of the dissociation limits of the low-lying electronic states of  $\text{NO}^{++}$  are shown in Table 9. The configuration sizes of the symmetries for  $\text{NO}^{++}$  are presented in Table 10.



These studies of the electronic structure of  $\text{NO}^+$  have included calculations of the potential energy curves to large internuclear separations where the adiabatic atomic connections can be made. These curves thus constitute a necessary data base for describing the charge exchange reaction:



This reaction is of significant concern in the overall DNA chemistry program of atmospheric modeling. The low energy ( $< 5$  eV) cross-section for this reaction is extremely difficult to obtain experimentally and the present studies should establish the background information needed for a theoretical description of this reaction. Such a program would be a natural follow-on to the present research program.

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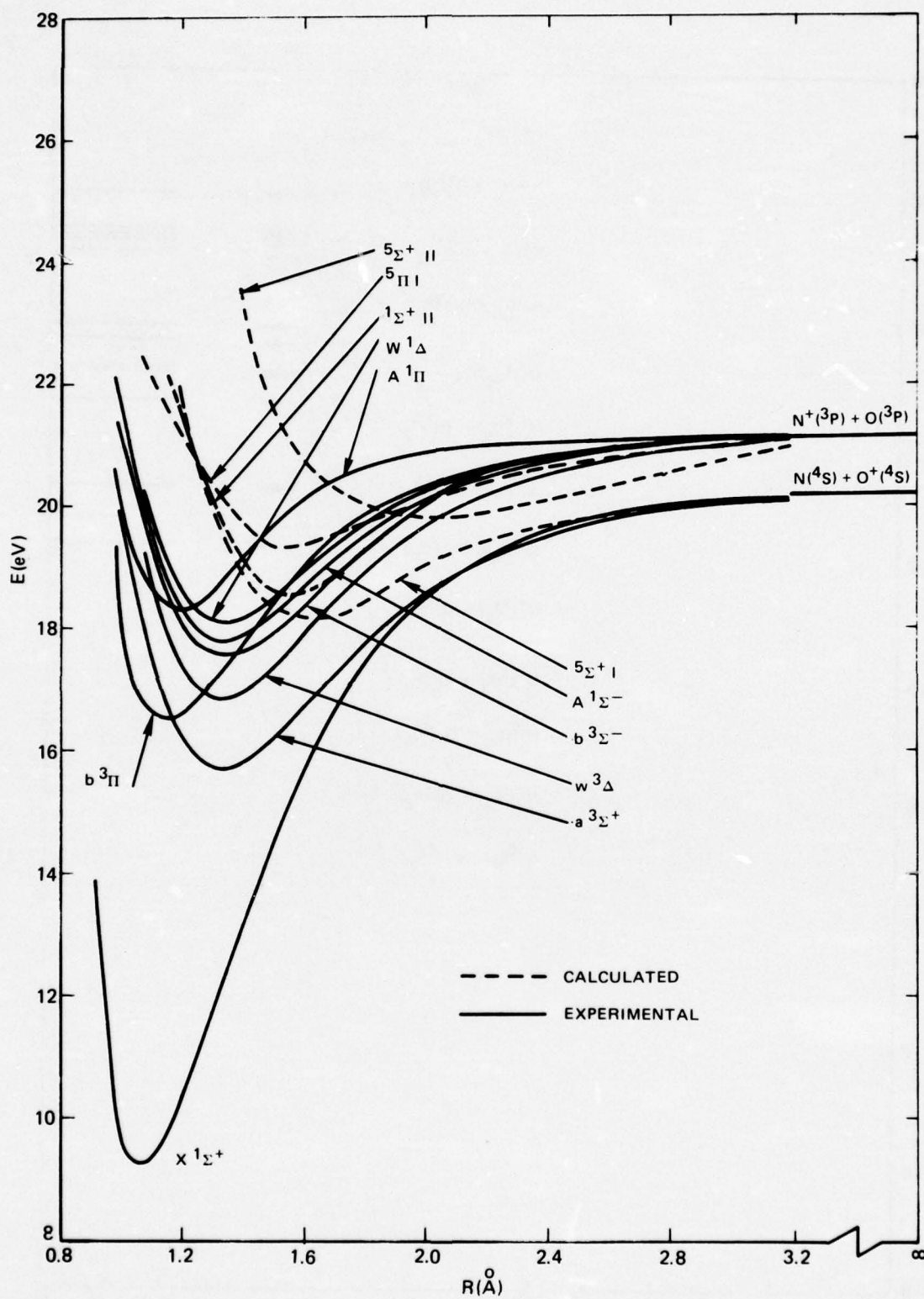


FIG. 1 LOW-LYING POTENTIAL ENERGY CURVES OF  $\text{NO}^+$

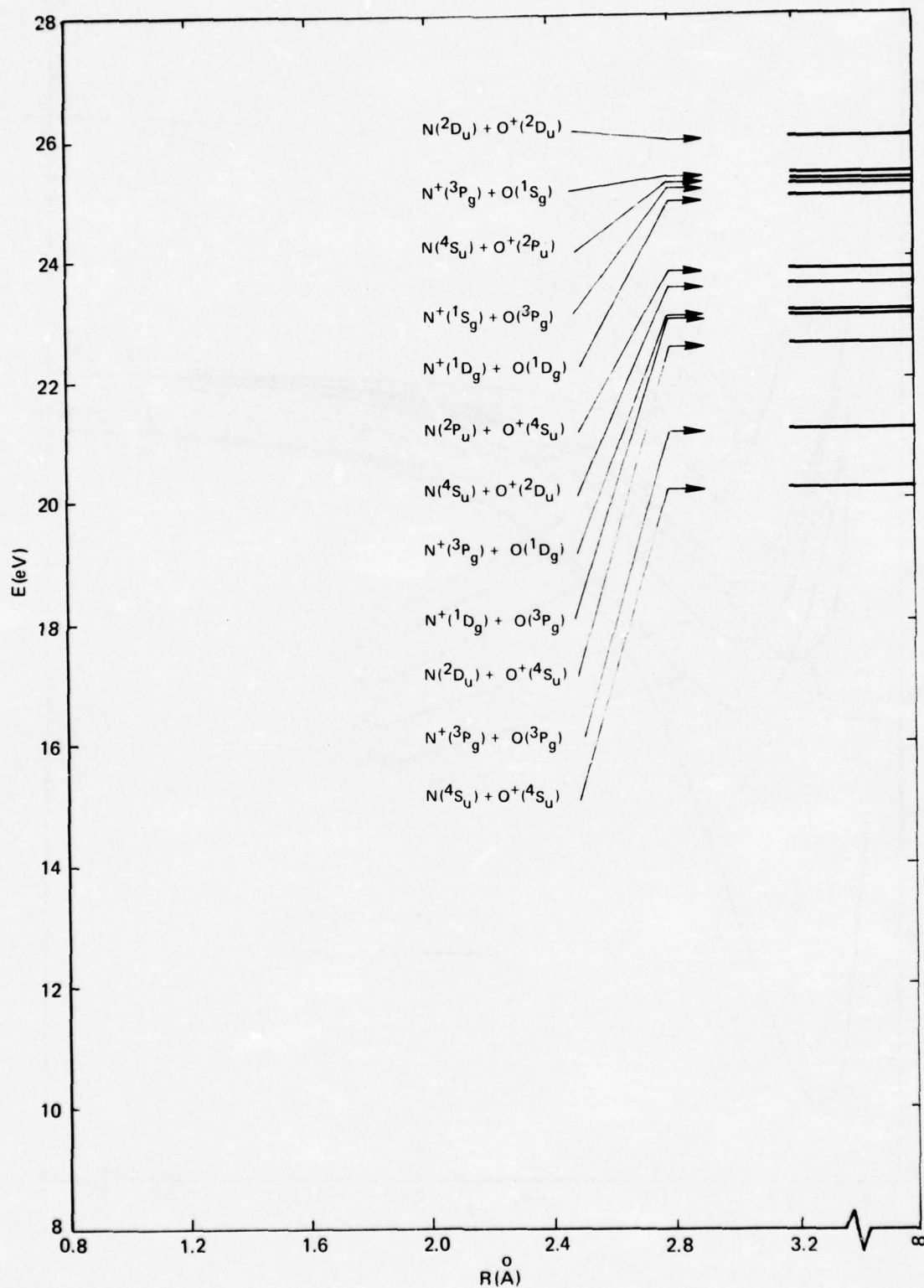


FIG. 2 LABELS FOR DISSOCIATION LIMITS

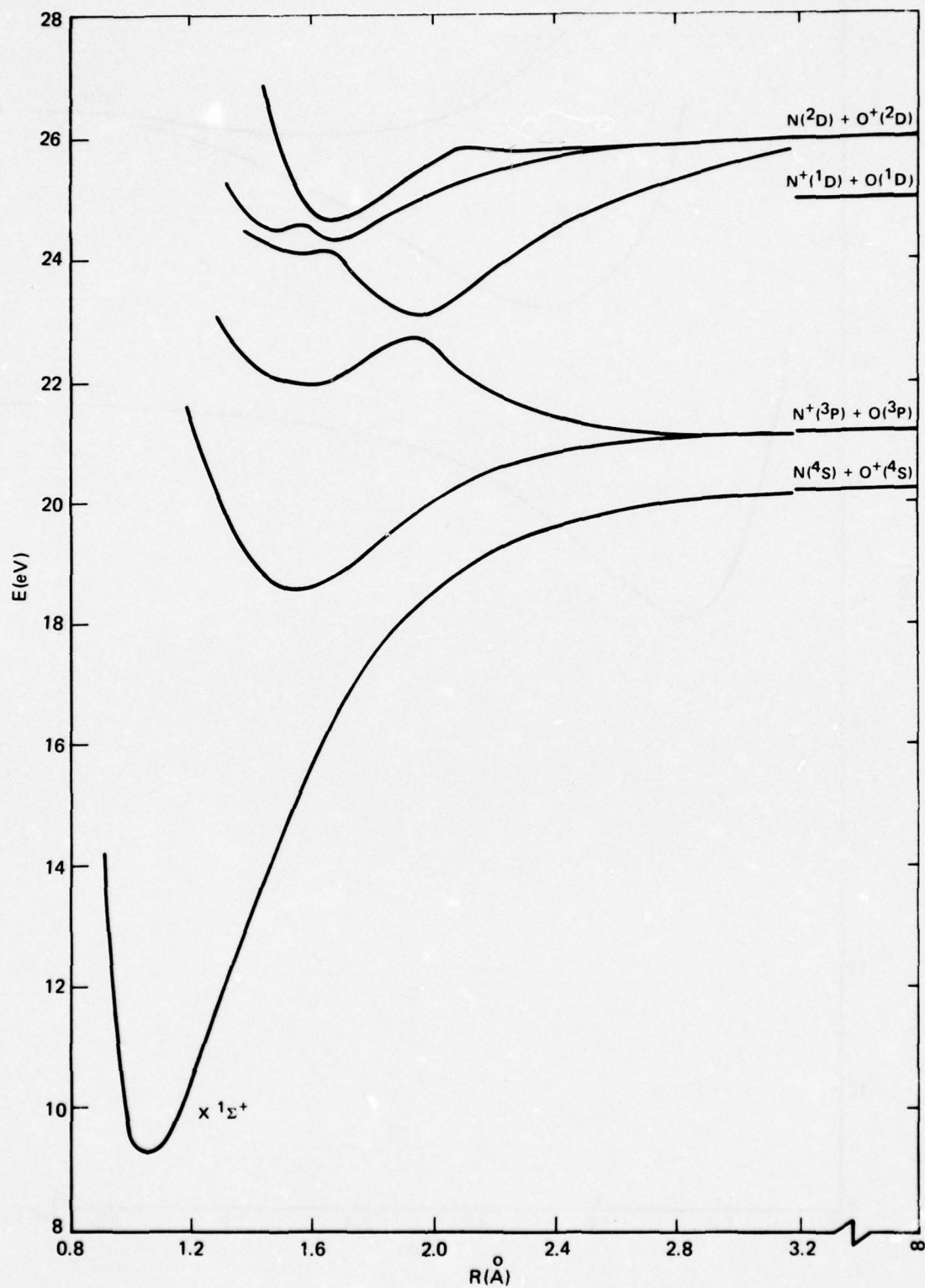


FIG. 3 POTENTIAL ENERGY CURVES FOR THE  $1\Sigma^+$  STATES OF  $\text{NO}^+$



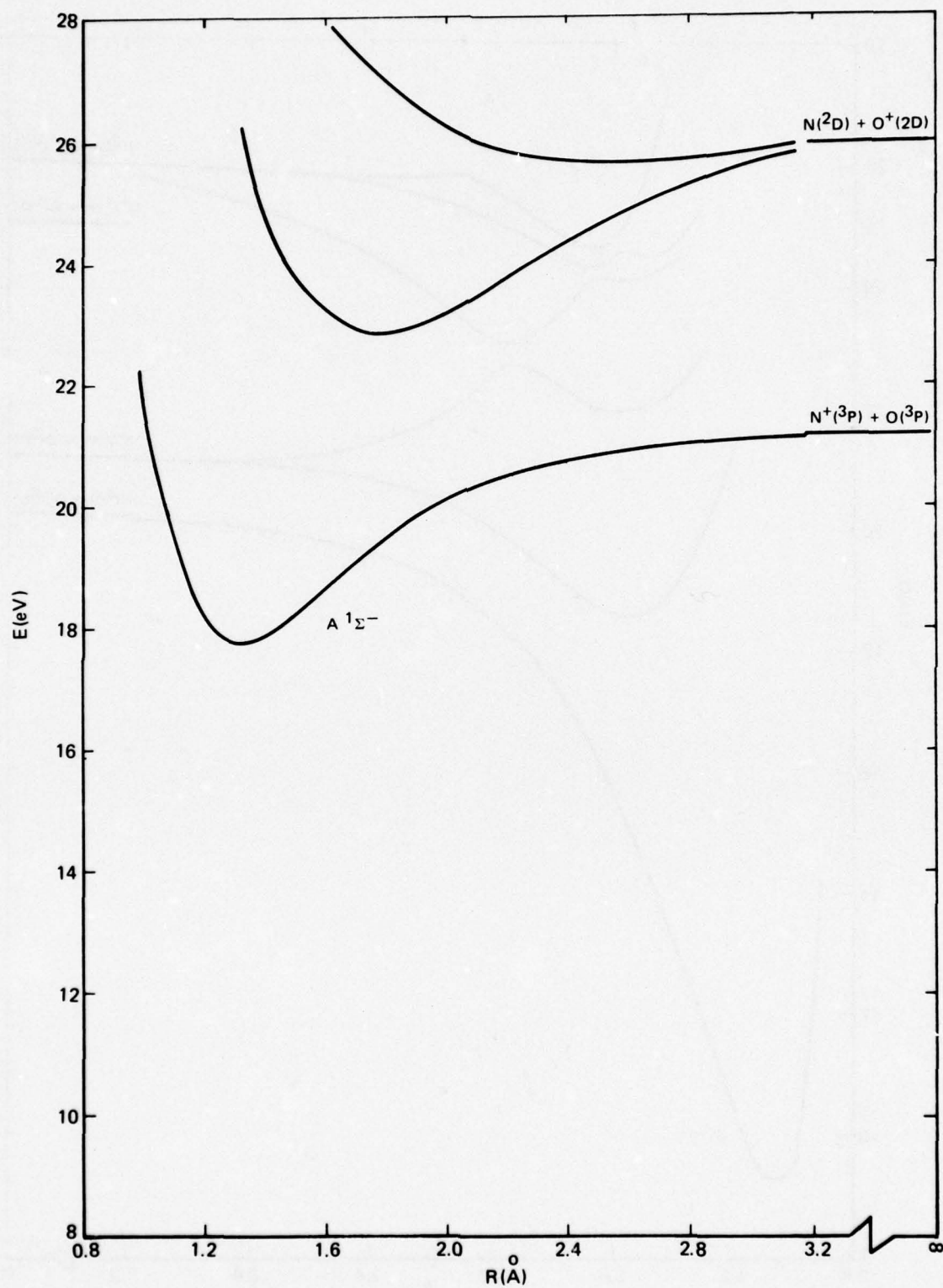


FIG. 4 POTENTIAL ENERGY CURVES FOR THE  $1\Sigma^-$  STATES OF  $\text{NO}^+$

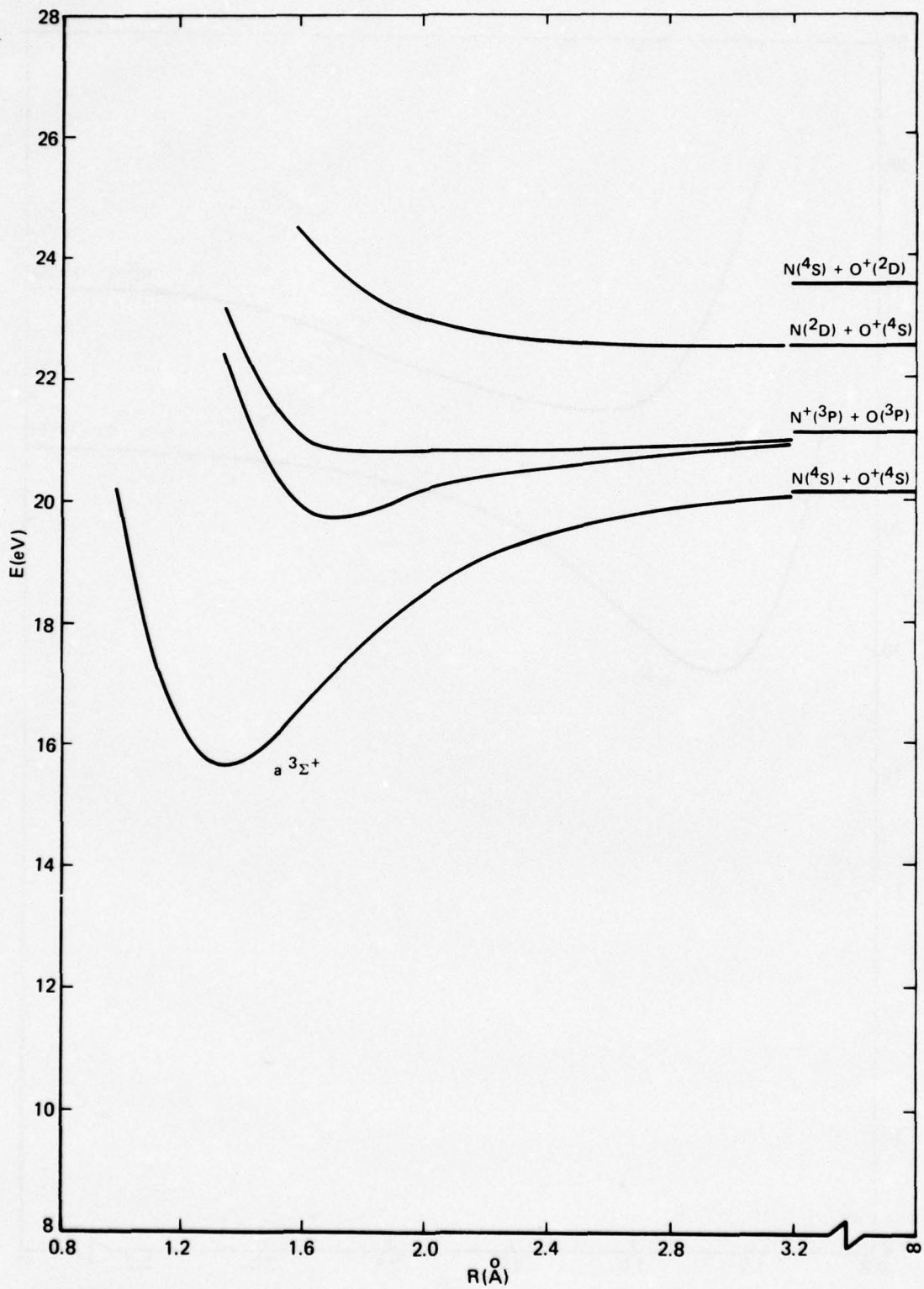


FIG. 5 POTENTIAL ENERGY CURVES FOR THE  $3\Sigma^+$  STATES OF  $\text{NO}^+$

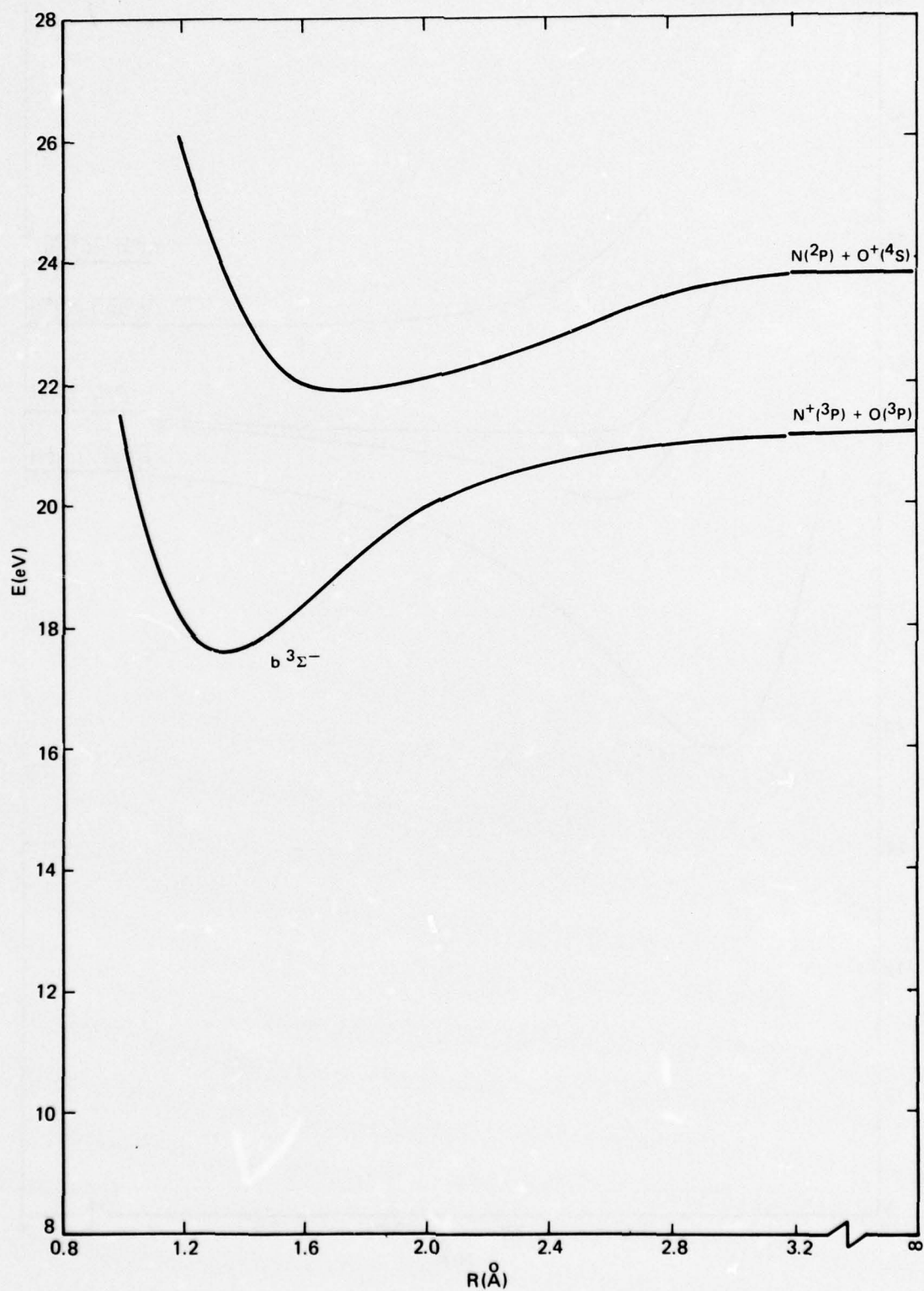


FIG. 6 POTENTIAL ENERGY CURVES FOR THE  $3\Sigma^-$  STATES OF  $\text{NO}^+$



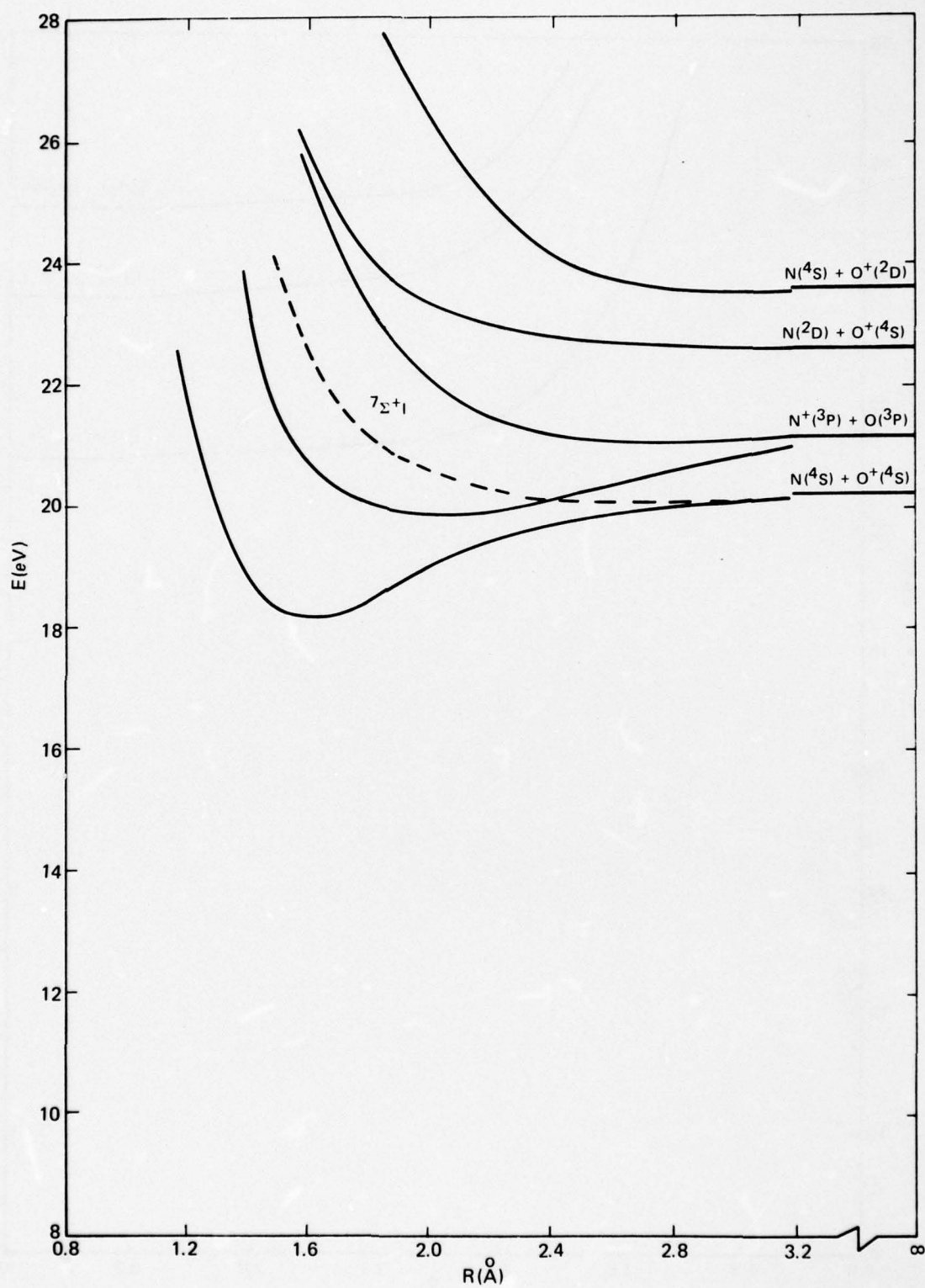


FIG. 7 POTENTIAL ENERGY CURVES FOR THE  $5\Sigma^+$  AND  $7\Sigma^+$  STATES OF  $\text{NO}^+$

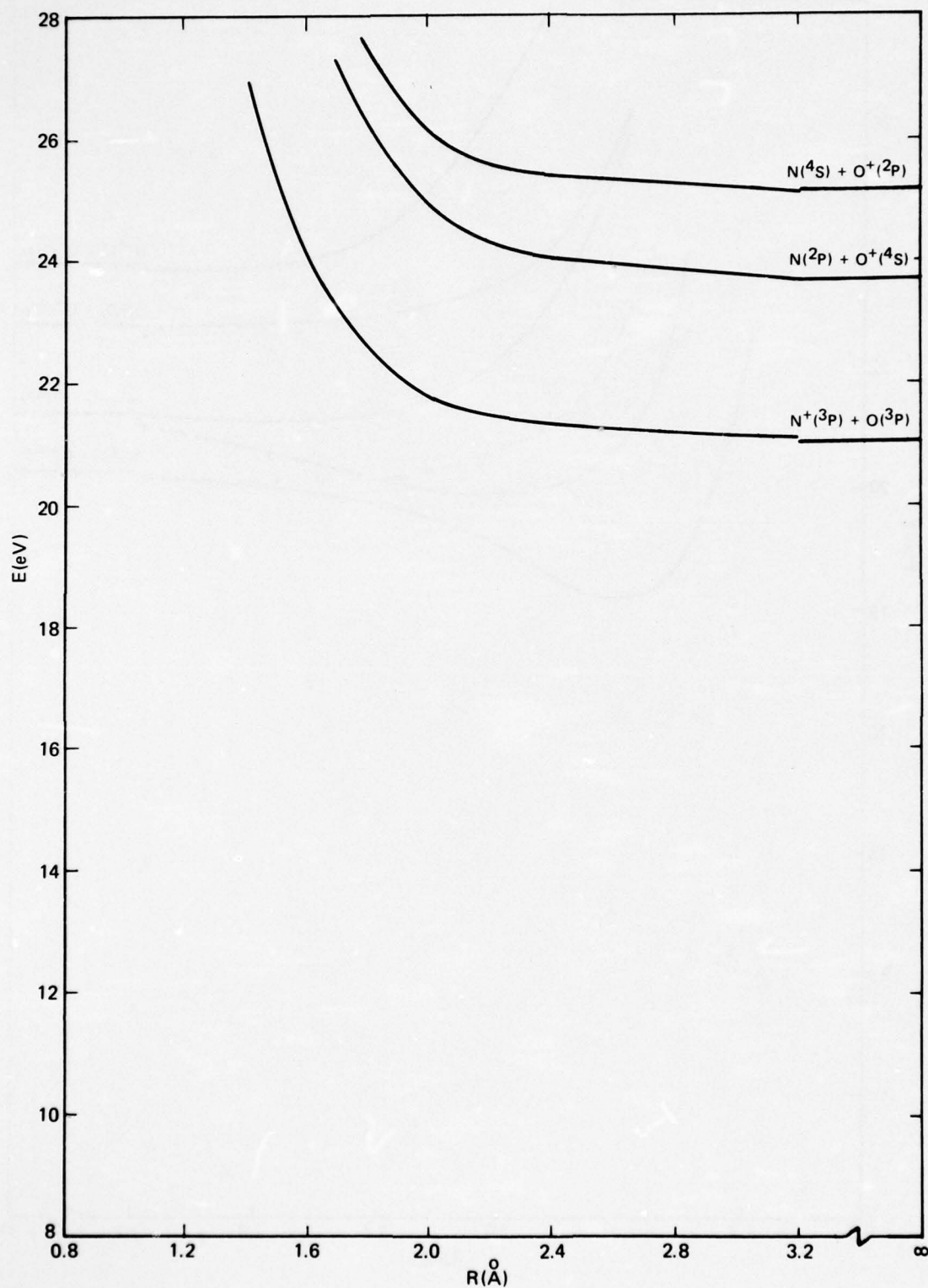


FIG. 8 POTENTIAL ENERGY CURVES FOR THE  $5\Sigma^-$  STATES OF  $\text{NO}^+$

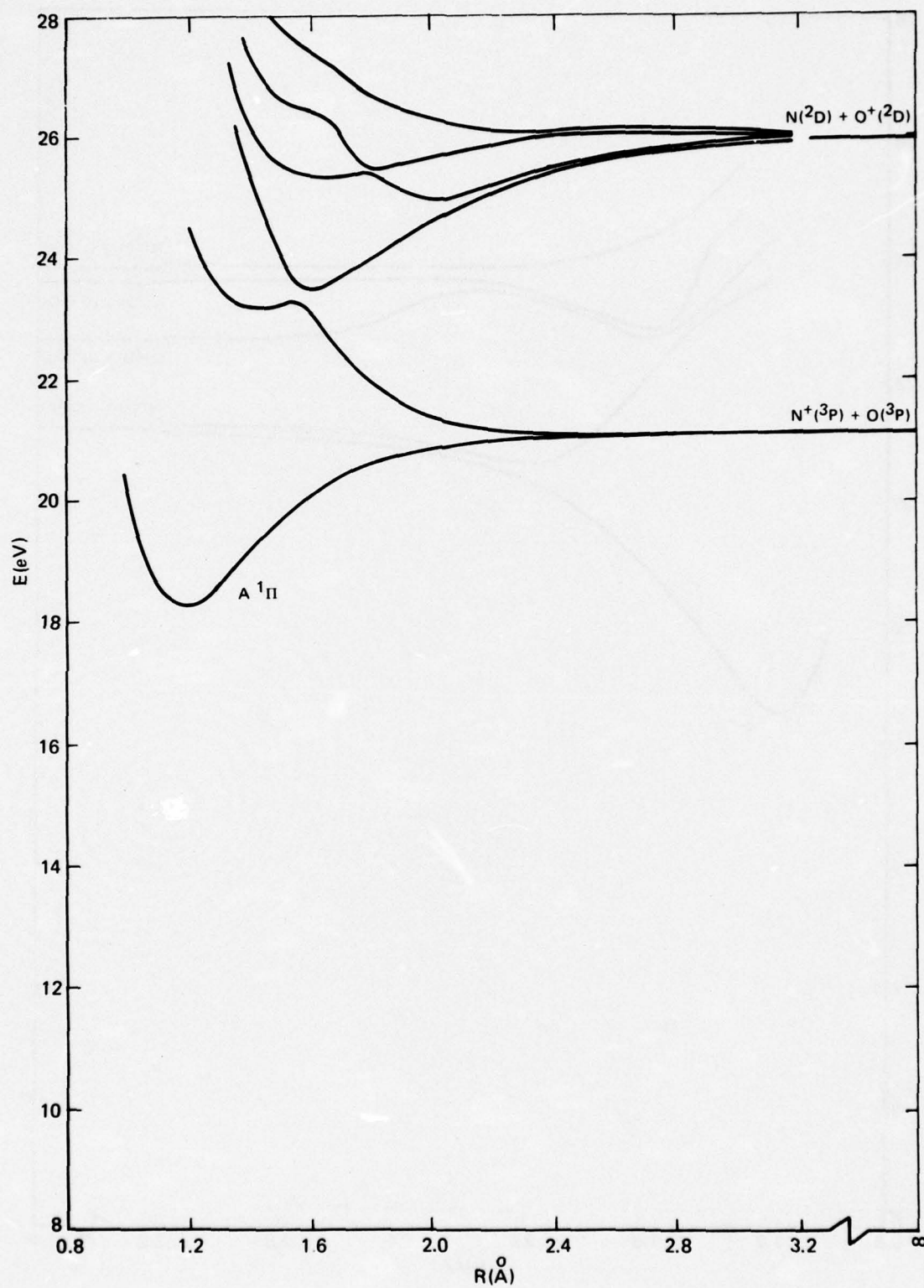


FIG. 9 POTENTIAL ENERGY CURVES FOR THE  $1\Pi$  STATES OF  $\text{NO}^+$



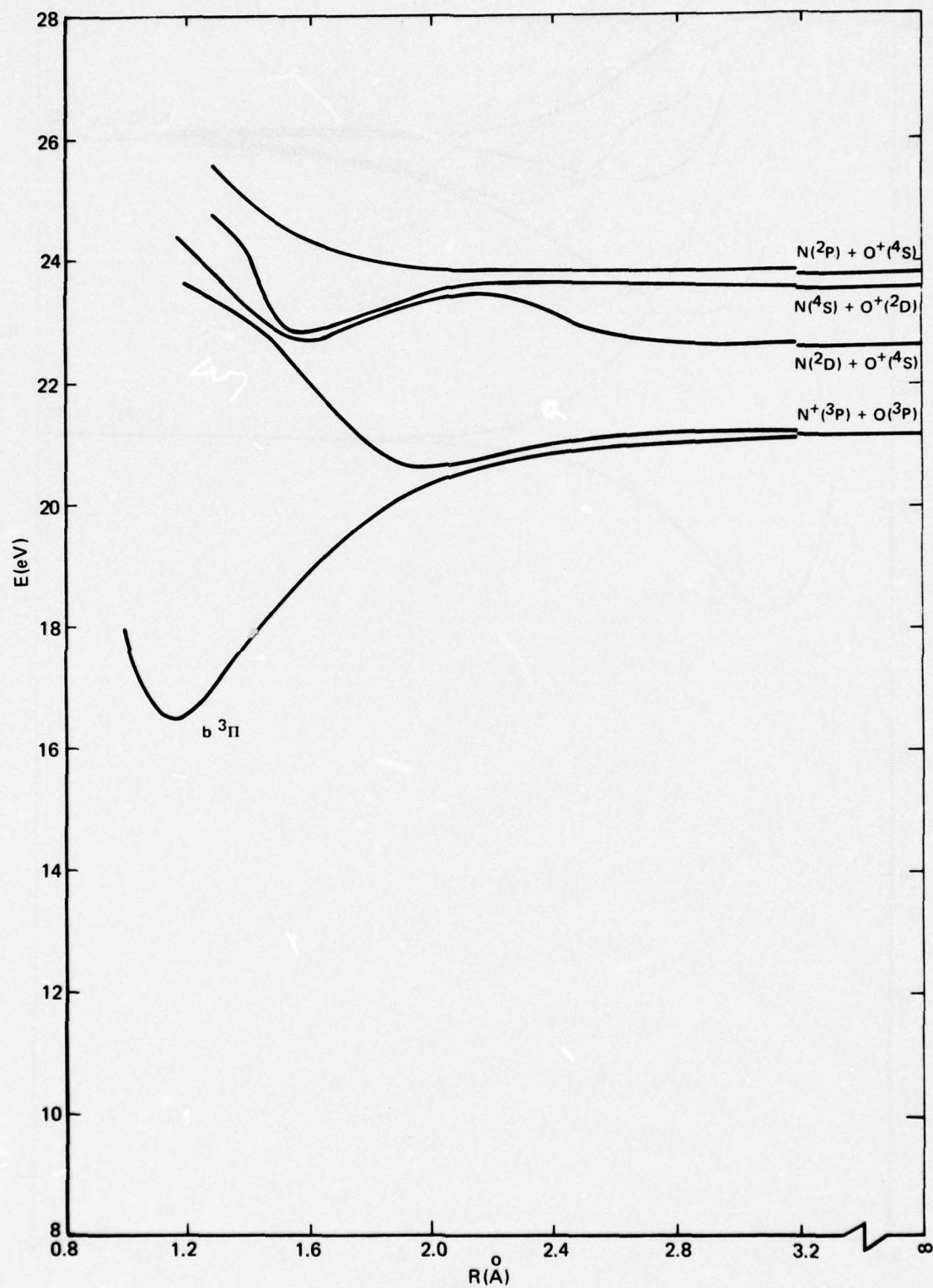


FIG. 10 POTENTIAL ENERGY CURVES FOR THE  $3\Pi$  STATES OF  $\text{NO}^+$

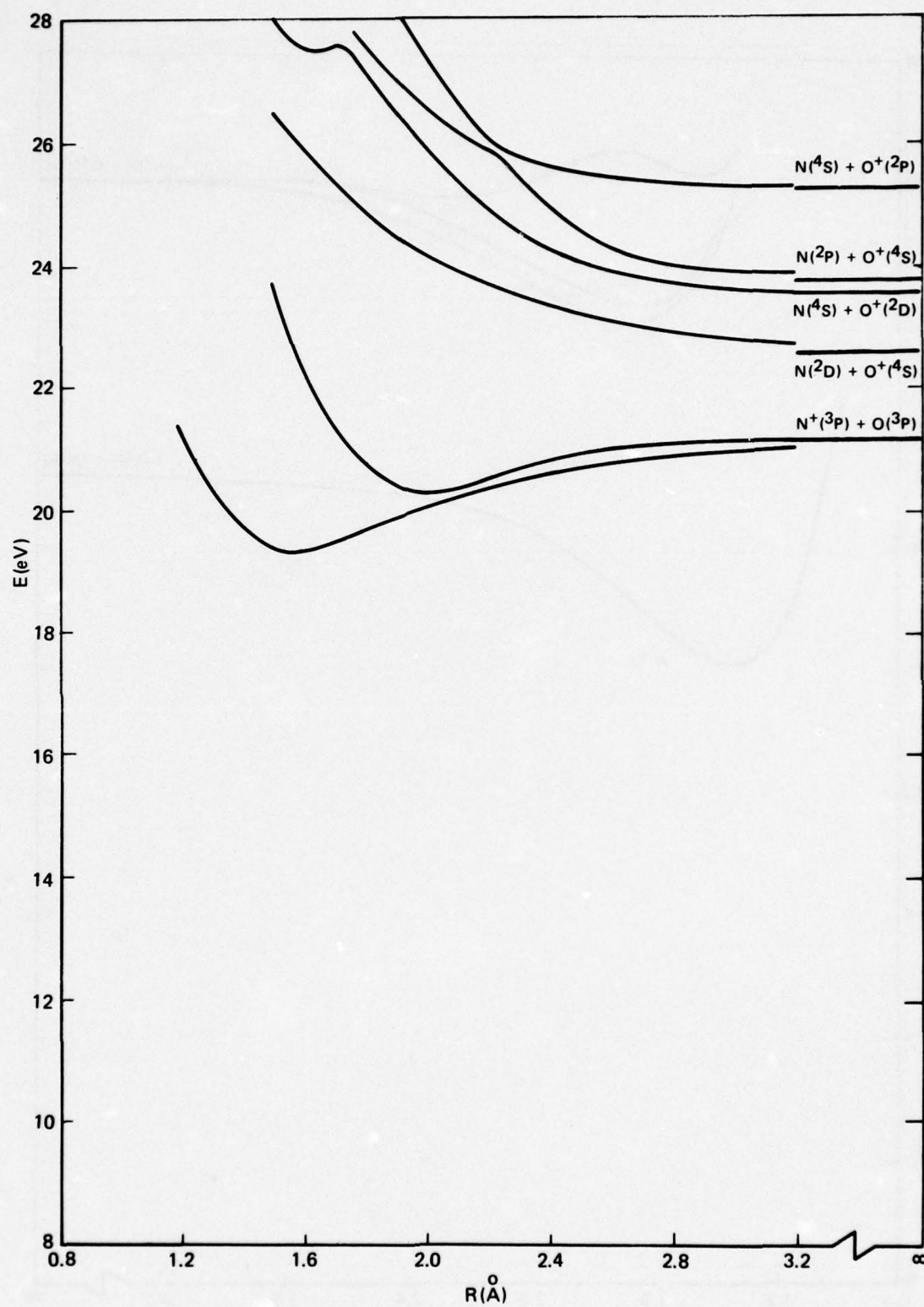


FIG. 11 POTENTIAL ENERGY CURVES FOR THE  $5\Pi$  STATES OF  $\text{NO}^+$

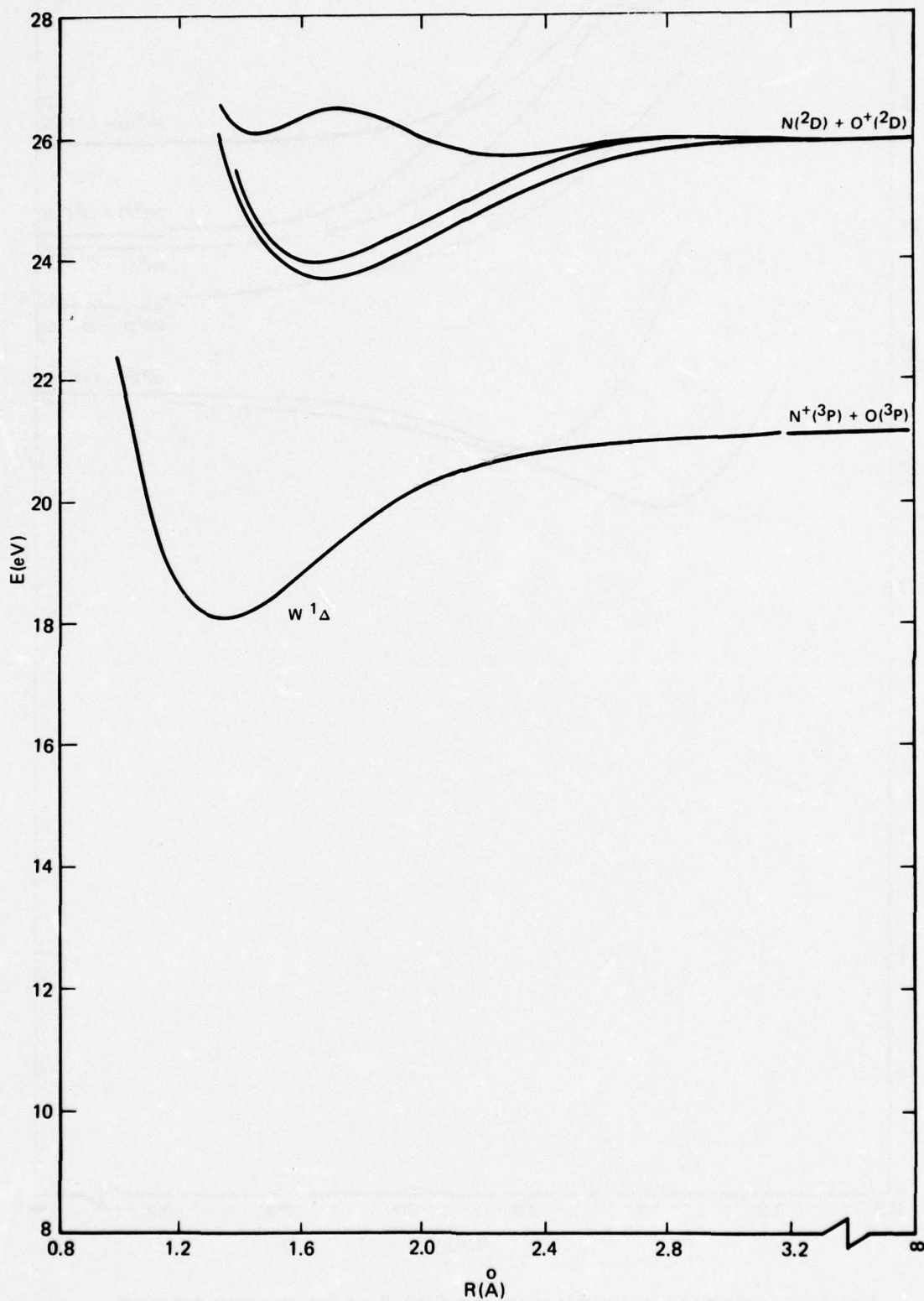


FIG. 12 POTENTIAL ENERGY CURVES FOR THE  $1\Delta$  STATES OF  $\text{NO}^+$



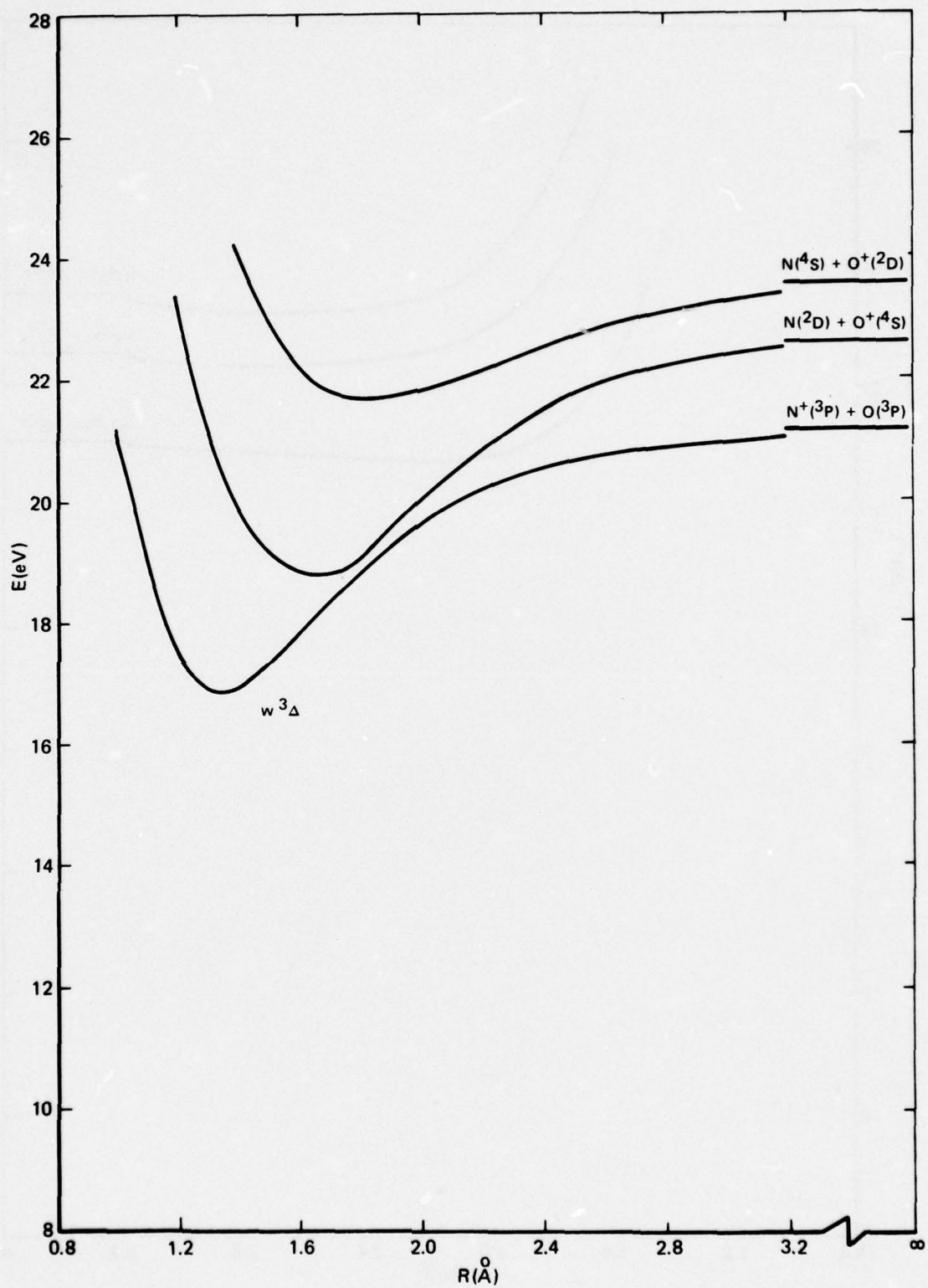


FIG. 13 POTENTIAL ENERGY CURVES FOR THE  $^3\Delta$  STATES OF  $\text{NO}^+$

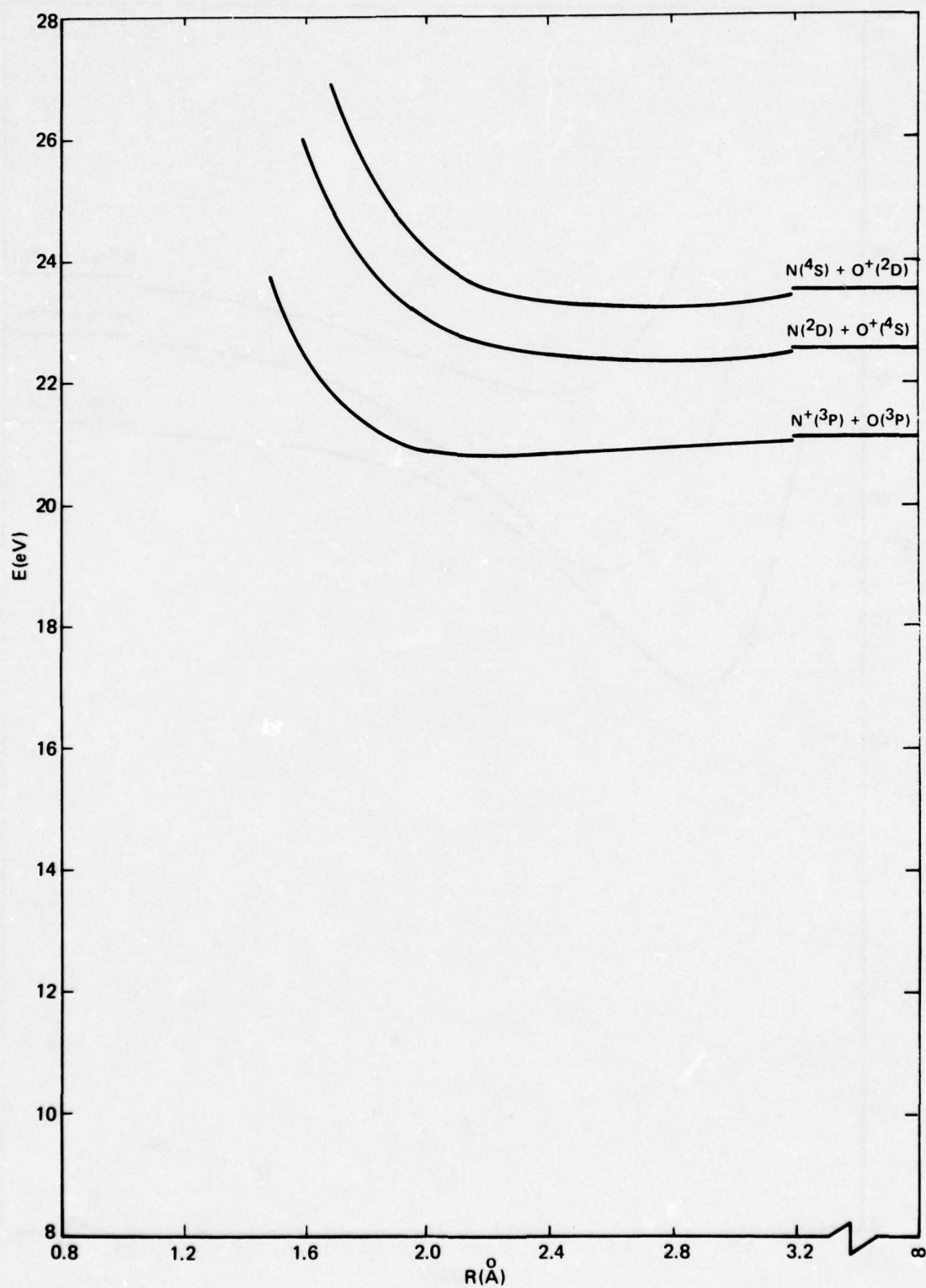


FIG. 14 POTENTIAL ENERGY CURVES FOR THE  $5\Delta$  STATES OF  $\text{NO}^+$

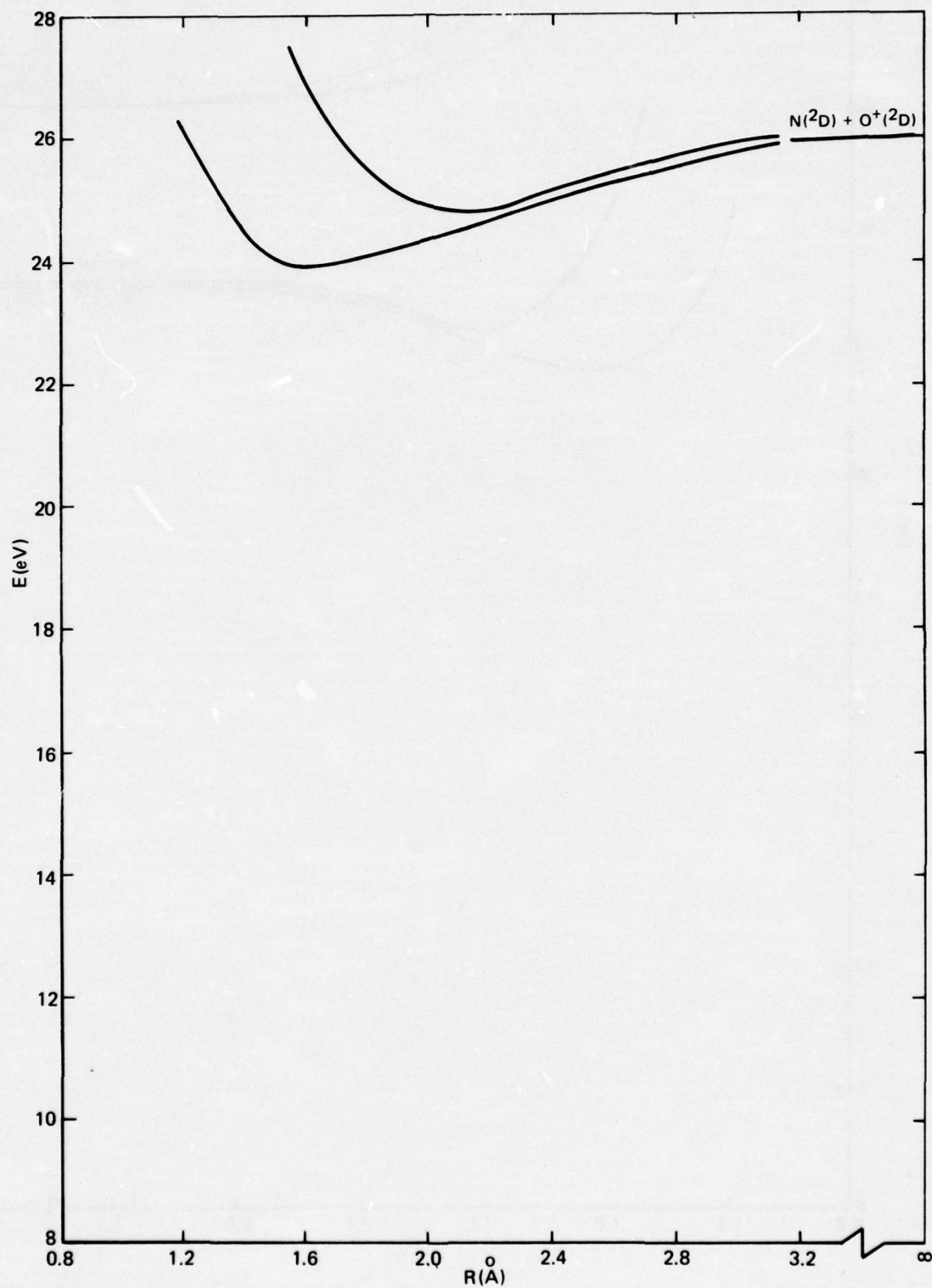


FIG. 15 POTENTIAL ENERGY CURVES FOR THE  $1\Phi$  STATES OF  $\text{NO}^+$



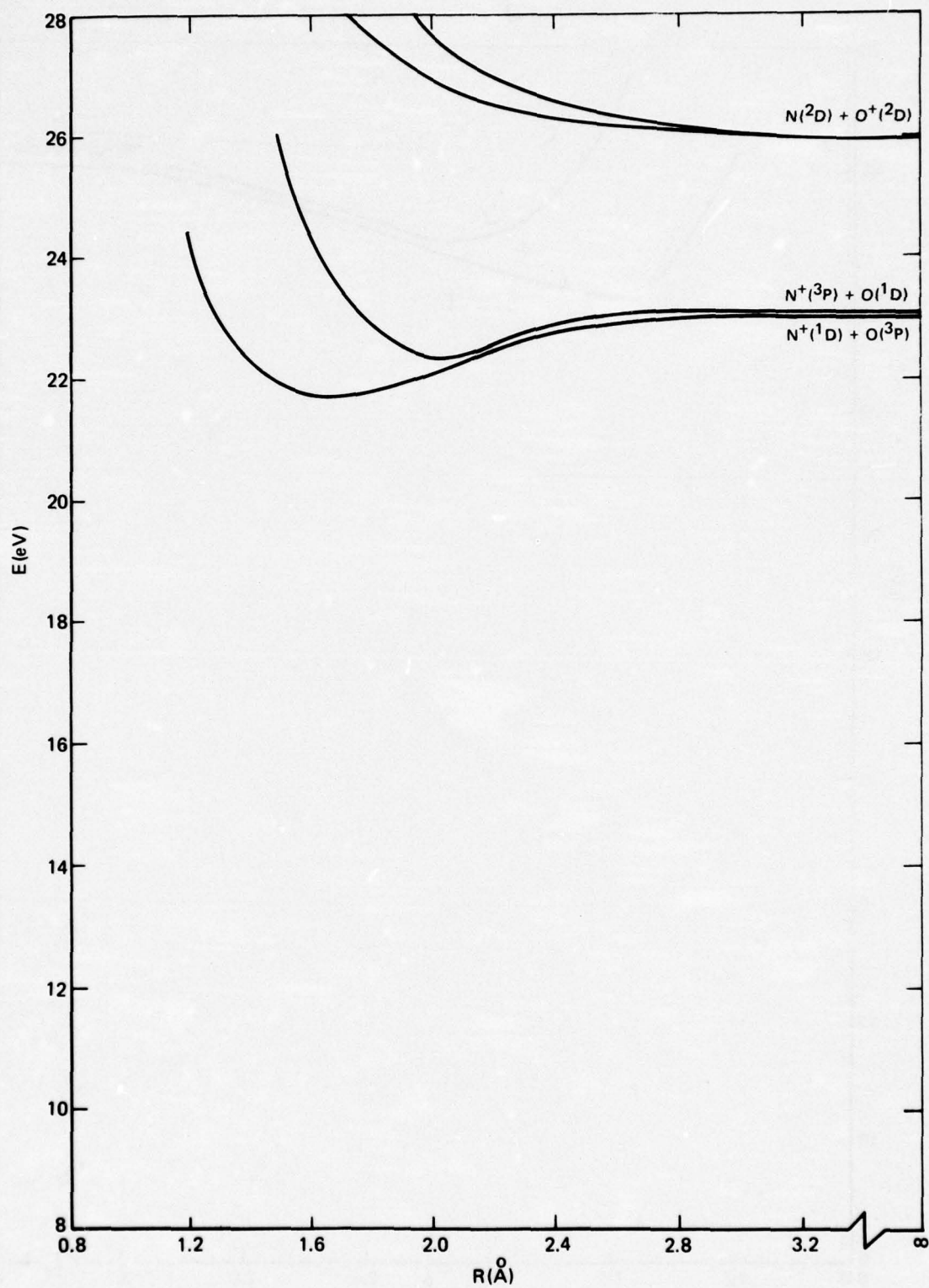


FIG. 16 POTENTIAL ENERGY CURVES FOR THE  $3\Phi$  STATES OF  $\text{NO}^+$

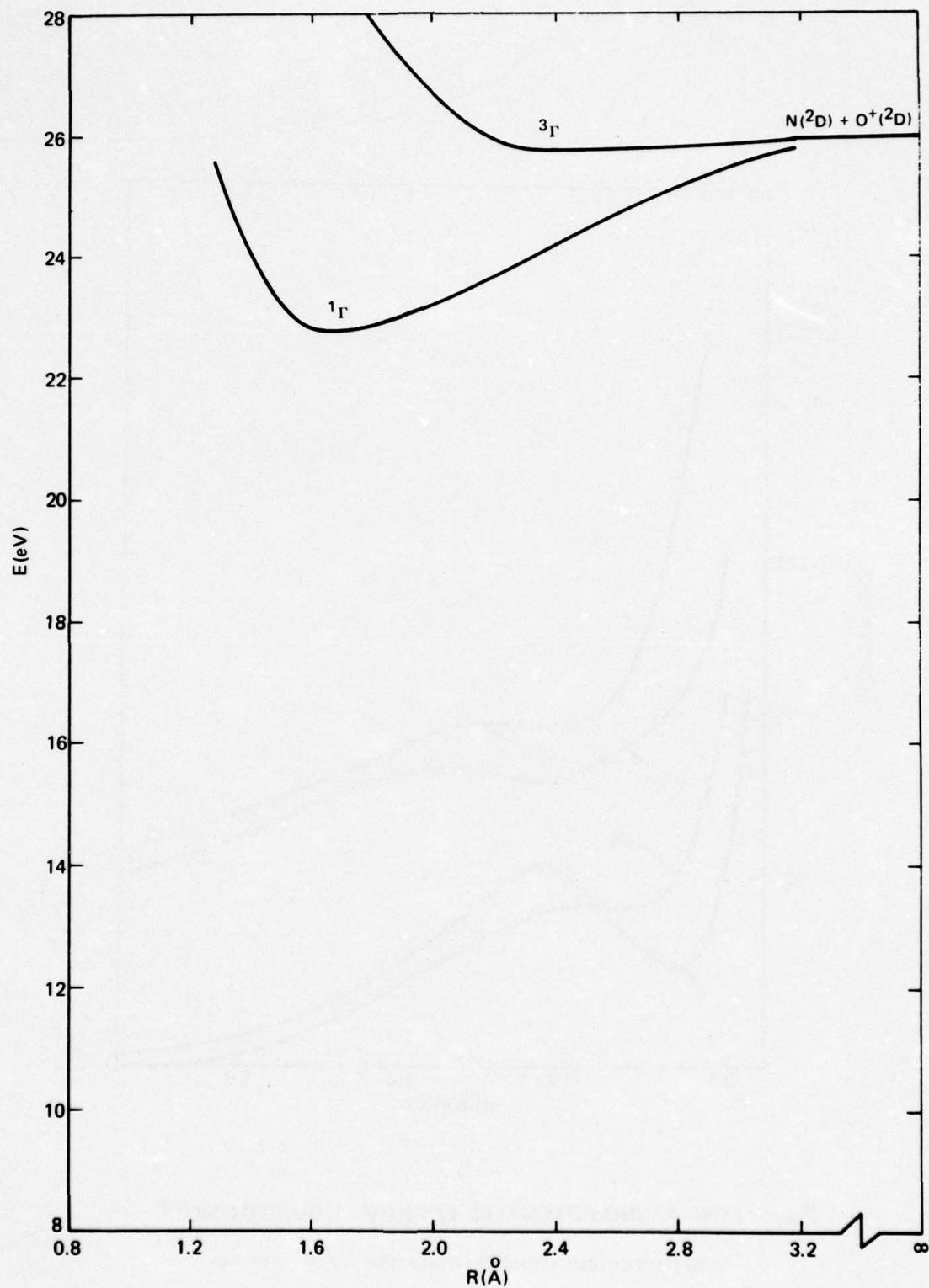
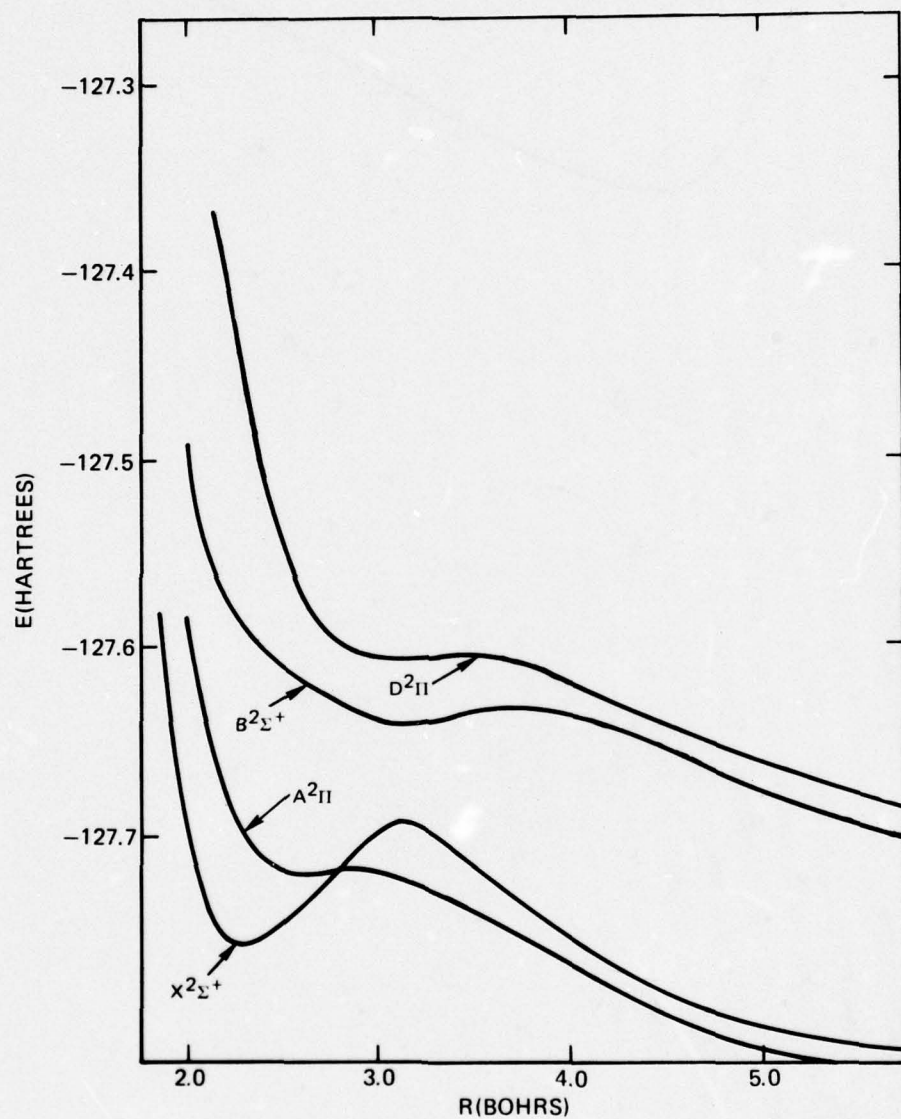


FIG. 17 POTENTIAL ENERGY CURVES FOR THE  $1\Gamma$  AND  $3\Gamma$  STATES OF  $\text{NO}^+$



**Fig. 18 LOW-LYING POTENTIAL ENERGY CURVES OF  $\text{NO}^{++}$**

(BASED ON CALCULATIONS OF THULSTRUP, ET. AL., REF. 48)



TABLE 1

LOW-LYING MOLECULAR STATES OF  $\text{NO}^+$  AND THEIR  
DISSOCIATION LIMITS

<u>Dissociation Limit</u> (Calculated Order)	<u>Molecular States</u>
$\text{N}(^4\text{S}_\text{u}) + \text{O}^+(^4\text{S}_\text{u})$	$^1\Sigma^+(1), ^3\Sigma^+(1), ^5\Sigma^+(1), ^7\Sigma^+(1)$
$\text{N}^+(^3\text{P}_\text{g}) + \text{O}(^3\text{P}_\text{g})$	$^1\Sigma^+(2), ^3\Sigma^+(2), ^5\Sigma^+(2),$ $^1\Sigma^-(1), ^3\Sigma^-(1), ^5\Sigma^-(1),$ $^1\Pi(2), ^3\Pi(2), ^5\Pi(2),$ $^1\Delta(1), ^3\Delta(1), ^5\Delta(1)$
$\text{N}(^2\text{D}_\text{u}) + \text{O}^+(^4\text{S}_\text{u})$	$^3\Sigma^+(1), ^5\Sigma^+(1), ^3\Pi(1),$ $^5\Pi(1), ^3\Delta(1), ^5\Delta(1)$
$\text{N}(^4\text{S}_\text{u}) + \text{O}^+(^2\text{D}_\text{u})$	$^3\Sigma^+(1), ^5\Sigma^+(1), ^3\Pi(1),$ $^5\Pi(1), ^3\Delta(1), ^5\Delta(1)$
$\text{N}(^2\text{P}_\text{u}) + \text{O}^+(^4\text{S}_\text{u})$	$^3\Sigma^-(1), ^5\Sigma^-(1), ^3\Pi(1),$ $^5\Pi(1)$
$\text{N}^+(^1\text{D}_\text{g}) + \text{O}(^3\text{P}_\text{g})$	$^3\Sigma^+(1), ^3\Sigma^-(2), ^3\Pi(3),$ $^3\Delta(2), ^3\Phi(1)$
$\text{N}(^4\text{S}_\text{u}) + \text{O}^+(^2\text{P}_\text{u})$	$^3\Sigma^-(1), ^5\Sigma^-(1),$ $^3\Pi(1), ^5\Pi(1)$

TABLE 1 (Cont'd)

LOW-LYING MOLECULAR STATES OF NO<sup>+</sup> AND THEIR  
DISSOCIATION LIMITS

<u>Dissociation Limit</u> (Calculated Order)	<u>Molecular States</u>
$N^+(^3P_g) + O(^1D_g)$	$^3\Sigma^+(1), ^3\Sigma^-(2), ^3\Pi(3),$ $^3\Delta(2), ^3\Phi(1)$
$N^+(^1S_g) + O(^3P_g)$	$^3\Sigma^-(1), ^3\Pi(1)$
$N(^2D_u) + O^+(^2D_u)$	$^1\Sigma^+(3), ^3\Sigma^+(3), ^1\Sigma^-(2),$ $^3\Sigma^-(2), ^1\Pi(4), ^3\Pi(4),$ $^1\Delta(3), ^3\Delta(3), ^1\Phi(2),$ $^3\Phi(2), ^1\Gamma(1), ^3\Gamma(1)$
$N^+(^1D_g) + O(^1D_g)$	$^1\Sigma^+(3), ^1\Sigma^-(2), ^1\Pi(4),$ $^1\Delta(3), ^1\Phi(2), ^1\Gamma(1)$
$N^+(^3P_g) + O(^1S_g)$	$^3\Sigma^-(1), ^3\Pi(1)$

TABLE 2

ENERGIES OF NITROGEN AND OXYGEN ATOMIC AND IONIC STATES REPRESENTING  
DISSOCIATION LIMITS OF LOW-LYING  $\text{NO}^+$  STATES

Atomic and Ionic States (Experimental order)	Total Energy (Hartrees)	Energy Relative to ${}^4\text{S}_u + {}^4\text{S}_u$ (eV)	
		Calc.	Exp.
$\text{N}({}^4\text{S}_u) + \text{O}^+({}^4\text{S}_u)$	-128.42277	0.000	0.000
$\text{N}^+({}^3\text{P}_g) + \text{O}({}^3\text{P}_g)$	-128.31777	2.857	0.916
$\text{N}({}^2\text{D}_u) + \text{O}^+({}^4\text{S}_u)$	-128.30317	3.255	2.383
$\text{N}^+({}^1\text{D}_g) + \text{O}({}^3\text{P}_g)$	-128.23804	5.027	2.815
$\text{N}^+({}^3\text{P}_g) + \text{O}({}^1\text{D}_g)$	-128.22386	5.413	2.883
$\text{N}({}^4\text{S}_u) + \text{O}^+({}^2\text{D}_u)$	-128.28190	3.833	3.325
$\text{N}({}^2\text{P}_u) + \text{O}^+({}^4\text{S}_u)$	-128.26192	4.377	3.575
$\text{N}^+({}^1\text{D}_g) + \text{O}({}^1\text{D}_g)$	-128.14412	7.583	4.782
$\text{N}^+({}^1\text{S}_g) + \text{O}({}^3\text{P}_g)$	-128.17437	6.759	4.968
$\text{N}({}^4\text{S}_u) + \text{O}^+({}^2\text{P}_u)$	-128.22932	5.264	5.016
$\text{N}^+({}^3\text{P}_g) + \text{O}({}^1\text{S}_g)$	-128.14286	7.617	5.105
$\text{N}({}^2\text{D}_u) + \text{O}^+({}^2\text{D}_u)$	-128.16229	7.088	5.708



TABLE 3  
CONFIGURATION SIZES AND NUMBER OF STATES FOR  
VCI CALCULATIONS OF VARIOUS SYMMETRIES FOR  $\text{NO}^+$

<u>Symmetry</u>	<u>No. Cfgs</u> (full CI)	<u>No. of States</u> (to and including $\text{N}^+3\text{P}_g + 0\ 1\text{s}_g$ dissociation limit)
$1_\Sigma$	296	9 (+), 5 (-)
$3_\Sigma$	392	10 (+), 11 (-)
$5_\Sigma$	126	5 (+), 3 (-)
$7_\Sigma$	10	1 (+)
$1_\Pi$	240	10
$3_\Pi$	328	18
$5_\Pi$	96	7
$7_\Pi$	8	-*
$1_\Delta$	142	7
$3_\Delta$	170	10
$5_\Delta$	43	3
$7_\Delta$	1	-**
$1_\Phi$	48	4
$3_\Phi$	56	4
$5_\Phi$	8	-***
$1_\Gamma$	10	2
$3_\Gamma$	6	1

\* First state dissociates to a high limit  $\text{N}^+(^5\text{S}_u) + 0(^3\text{P}_g)$

\*\* First state dissociates to a high limit  $\text{N}(^4\text{P}_g) + 0(^4\text{P}_g)$

\*\*\* First state dissociates to a high limit  $\text{N}^+(^3\text{D}_u) + 0(^3\text{P}_g)$

TABLE 4

Experimental Constants for Low-Lying Bound States of NO<sup>+</sup>

State/Constant	Energy (eV) Above X <sup>2</sup> Π(NO) <sup>a</sup>	r <sub>e</sub> (Å) <sup>a</sup>	w <sub>e</sub> (cm <sup>-1</sup> ) <sup>a</sup>	w <sub>e</sub> X <sub>e</sub> (cm <sup>-1</sup> ) <sup>b</sup>	α <sub>e</sub> (cm <sup>-1</sup> ) <sup>b</sup>	B <sub>e</sub> (cm <sup>-1</sup> ) <sup>b</sup>
X <sup>1</sup> Σ <sup>+</sup>	9.3	1.06	2370	16 <sup>a</sup>	.020	2.002
A <sup>1</sup> Σ <sup>-</sup>	17.8	1.34	1260	15	.015	1.257
a <sup>3</sup> Σ <sup>+</sup>	15.7	1.34	1300	12	.012	1.257
b <sup>3</sup> Σ <sup>-</sup>	17.6	1.34	1200	13	.014	1.251
A <sup>1</sup> Π	18.3	1.19	1609	23 <sup>a</sup>	.024	1.587
b <sup>3</sup> Π	16.5	1.16	1690	20	.019	1.677
W <sup>1</sup> Δ	18.1	1.34	1250	16	.016	1.257
W <sup>3</sup> Δ	16.9	1.34	1300	13	.012	1.257

<sup>a</sup> Based on photoelectron spectra of Thulstrup, et al. (Ref. 48).<sup>b</sup> Calculated using experimental constants of Thulstrup, et al. (Ref. 48).

TABLE 5

Calculated Oscillator Strengths ( $f_{v',v''}$ ) for  
the Vibrational-Rotational Transition of  
 $\text{NO}^+ (X^1\Sigma^+ - X^1\Sigma^+)$

$v'/v''$	0	1	2	3	4	5
0						
1	7.072-06					
2	6.163-08	1.408-05				
3	1.936-09	1.828-07	2.100-05			
4	1.293-10	6.714-09	3.686-07	2.775-05		
5	1.295-12	7.394-10	1.455-08	6.136-07	3.435-05	
6	2.333-13	2.388-11	1.535-09	2.636-08	9.151-07	4.078-05
7	1.109-12	1.410-11	8.597-11	2.548-09	4.254-08	1.272-06
8	7.310-13	9.871-12	3.187-11	1.601-10	3.888-09	6.401-08
9	8.058-12	2.088-12	6.418-11	4.181-11	2.709-10	6.195-09
10	5.324-12	3.967-12	1.900-11	1.304-10	1.415-11	3.694-10

$v'/v''$	6	7	8	9	10
0					
1					
2					
3					
4					
5					
6					
7	4.703-05				
8	1.691-06	5.305-05			
9	8.944-08	2.176-06	5.884-05		
10	9.491-09	1.191-07	2.729-06	6.435-05	



TABLE 6

Calculated Einstein Coefficients ( $A_{v'v''}$ ,  $\text{sec}^{-1}$ )  
for the  $X^1\Sigma^+ - X^1\Sigma^+$  System of  $\text{NO}^+$

$v'/v''$	0	1	2	3	4	5
0						
1	2.592+01					
2	8.912-01	5.019+01				
3	6.211-02	2.569+00	7.273+01			
4	7.272-03	2.093-01	5.034+00	9.340+01		
5	1.121-04	4.039-02	4.406-01	8.140+00	1.123+02	
6	2.868-05	2.009-03	8.146-02	7.754-01	1.179+01	1.293+02
7	1.829-04	1.683-03	7.023-03	1.313-01	1.214+00	1.590+01
8	1.552-04	1.581-03	3.695-03	1.270-02	1.944-01	1.773+00
9	2.133-03	4.303-04	9.975-03	4.703-03	2.084-02	3.004-01
10	1.714-03	1.019-03	3.800-03	1.966-02	1.544-03	2.756-02
$v'/v''$	6	7	8	9	10	
0						
1						
2						
3						
4						
5						
6						
7	1.447+02					
8	2.050+01	1.583+02				
9	2.402+00	2.558+01	1.702+02			
10	4.463-01	3.100+00	3.108+01	1.804+02		

TABLE 7

Total Integrated Absorption Coefficient  
for  $\text{NO}^+$  ( $\times 10^3$ )

Temperature (°K)	Absorption Coefficient, $\text{cm}^{-2} \text{ atm}^{-1}$				
	<u>Fundamental</u>	<u>First Overtone</u>	<u>Second Overtone</u>	<u>Third Overtone</u>	<u>Total</u>
100.	168.278	1.467	0.046	0.003	169.794
273.16	168.278	1.467	0.046	0.003	169.794
300.	168.278	1.467	0.046	0.003	169.794
500.	168.276	1.470	0.046	0.003	169.795
1000.	168.223	1.569	0.050	0.004	169.846
1500.	168.087	1.811	0.061	0.005	169.964
2000.	167.886	2.133	0.076	0.007	170.102
2500.	167.631	2.501	0.095	0.009	170.236
3000.	167.328	2.894	0.118	0.012	170.352
4000.	166.590	3.730	0.172	0.013	170.510
5000.	165.682	4.606	0.236	0.026	170.550
8000.	161.637	7.260	0.461	0.057	169.415
10000.	157.481	8.776	0.604	0.077	166.938

TABLE 8

Low-Lying Molecular States of  $\text{NO}^{++}$  and Their  
Dissociation Limits

<u>Dissociation Limit</u> (Experimental Order)	<u>Molecular States</u>
$\text{N}^+(^3\text{P}_g) + \text{O}^+(^4\text{S}_u)$	$^2\Sigma^+(1), ^4\Sigma^+(1), ^6\Sigma^+(1),$ $^2\Pi(1), ^4\Pi(1), ^6\Pi(1)$
$\text{N}^{++}(^2\text{P}_u) + \text{O}(^3\text{P}_g)$	$^2\Sigma^-(2), ^4\Sigma^-(2), ^2\Sigma^+(1), ^4\Sigma^+(1)$ $^2\Pi(2), ^4\Pi(2), ^2\Delta(1), ^4\Delta(1)$ $^4\Sigma^-(1), ^4\Pi(1), ^4\Delta(1)$
$\text{N}^+(^1\text{D}_g) + \text{O}^+(^4\text{S}_u)$	$^2\Sigma^-(1), ^4\Sigma^-(1), ^2\Sigma^+(2), ^4\Sigma^+(2),$ $^2\Pi(3), ^4\Pi(3), ^2\Delta(2), ^4\Delta(2),$ $^2\Phi(1), ^4\Phi(1)$
$\text{N}^{++}(^2\text{P}_u) + \text{O}(^1\text{D}_g)$	$^2\Sigma^-(1), ^2\Sigma^+(2), ^2\Pi(3), ^2\Delta(2),$ $^2\Phi(1),$ $^4\Sigma^-(1)$
$\text{N}^+(^1\text{S}_g) + \text{O}^+(^4\text{S}_u)$	$^2\Sigma^-(2), ^4\Sigma^-(2), ^2\Sigma^+(1), ^4\Sigma^+(1),$ $^2\Pi(2), ^4\Pi(2), ^2\Delta(1), ^4\Delta(1)$
$\text{N}^+(^3\text{P}_g) + \text{O}^+(^2\text{P}_u)$	$^2\Sigma^-(3), ^2\Sigma^+(2), ^2\Pi(4), ^2\Delta(3),$ $^2\Phi(2), ^2\Gamma(1)$
$\text{N}^{++}(^2\text{P}_u) + \text{O}(^1\text{S}_g)$	$^2\Sigma^+(1), ^2\Pi(1)$
$\text{N}^+(^5\text{S}_u) + \text{O}^+(^4\text{S}_u)$	$^2\Sigma^+(1), ^4\Sigma^+(1), ^6\Sigma^+(1), ^8\Sigma^+(1)$
$\text{N}^+(^1\text{D}_g) + \text{O}^+(^2\text{P}_u)$	$^2\Sigma^-(1), ^2\Sigma^+(2), ^2\Pi(3), ^2\Delta(2),$ $^2\Phi(1)$
$\text{N}(^4\text{S}_u) + \text{O}^{++}(^3\text{P}_g)$	$^2\Sigma^+(1), ^4\Sigma^+(1), ^6\Sigma^+(1), ^2\Pi(1),$ $^4\Pi(1), ^6\Pi(1)$



TABLE 9

Energies of Nitrogen and Oxygen Ionic States Representing  
Dissociation Limits of Low-Lying  $\text{NO}^{++}$  States

Ionic States (Experimental Order)	Total Energy (Hartrees)	Energy Relative to $\text{N}^+(^3\text{P}_g) + \text{O}^+(^4\text{S}_u)$ eV	
		Calc.	Exp.
$\text{N}^+(^3\text{P}_g) + \text{O}^+(^4\text{S}_u)$	-127.93207	0.000	0.000
$\text{N}^{++}(^2\text{P}_u) + \text{O}(^3\text{P}_g)$	$(-127.20712)^*$	$(19.727)^*$	1.452
$\text{N}^+(^1\text{D}_g) + \text{O}^+(^4\text{S}_u)$	-127.85233	2.170	1.899
$\text{N}^+(^3\text{P}_g) + \text{O}^+(^2\text{D}_u)$	-127.79139	3.828	3.325
$\text{N}^{++}(^2\text{P}_u) + \text{O}(^1\text{D}_g)$	$(-127.1132)^*$	$(22.283)^*$	3.419
$\text{N}^+(^1\text{S}_g) + \text{O}^+(^4\text{S}_u)$	-127.76201	4.628	4.052
$\text{N}^+(^3\text{P}_g) + \text{O}^+(^2\text{P}_u)$	-127.69747	6.384	5.016
$\text{N}^+(^1\text{D}_g) + \text{O}^+(^2\text{D}_u)$	-127.70185	6.265	5.223
$\text{N}^{++}(^2\text{P}_u) + \text{O}(^1\text{S}_g)$	$(-127.03220)^*$	$(24.487)^*$	5.641
$\text{N}^+(^5\text{S}_u) + \text{O}^+(^4\text{S}_u)$	-127.84272	2.431	5.847
$\text{N}^+(^1\text{D}_g) + \text{O}^+(^2\text{P}_u)$	-127.60793	8.320	7.015
$\text{N}(^4\text{S}_u) + \text{O}^{++}(^3\text{P}_g)$	$(-127.09326)^*$	$(22.825)^*$	7.002

\* non-optimized calculation

TABLE 10

Configuration Sizes and Number of States for VCI  
Calculations of Various Symmetries for  $\text{NO}^{++}$

<u>Symmetry</u>	<u>No. Cfgs.</u>	<u>No. of States (to and including <math>\text{N}(^4\text{S}_u + \text{O}^{++}(^3\text{P}_g)</math> dissociation limit)</u>
$2\Gamma$	20	1
$4\Phi$	44	1
$2\Phi$	102	5
$4\Delta$	152	5
$2\Delta$	276	11
$6\Pi$	52	2
$4\Pi$	292	10
$2\Pi$	486	20
$8\Sigma^+$	4	1
$6^+ \Sigma$	68	3
$4^{+,-} \Sigma$	360	7(+), 7(-)
$2^{+,-} \Sigma$	584	14(+), 10(-)

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